OPCW

Scientific Advisory Board

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SUMMARY OF THE SECOND MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON ARTIFICIAL INTELLIGENCE 24 – 26 JUNE 2025

1. AGENDA ITEM ONE – Opening of the meeting and adoption of the agenda

1.1 The Temporary Working Group (TWG) on Artificial Intelligence (AI) of the Scientific Advisory Board (SAB) held its second meeting from 24 to 26 June 2025 at the operational base of the China-BRICS[1] Artificial Intelligence Development and Cooperation Center (BRICS AI Center) in Shanghai, China. The meeting was chaired by Dr Catharina Müller-Buschbaum on behalf of the SAB, with Prof. Hajar Mousannif as Vice-Chairperson.

1.2 Dr Müller-Buschbaum and Prof. Mousannif opened the meeting by welcoming the TWG members and external speakers. In particular, they expressed thanks to Group member Dr Tongning Wu and his organisations—the China Academy of Information and Communications Technology (CAICT) and the BRICS AI Center—for hosting the meeting and welcoming the TWG members. The Secretary to the SAB provided the Group with additional logistical and organisational information. The Chairperson then invited all participants to introduce themselves and a list of participants appears in the Annex to this report.

1.3 As no objections or comments were raised in response to the proposed programme of work during the three days of the meeting, the TWG adopted the following agenda for its second meeting:

1. Opening of the meeting and adoption of the agenda
2. Welcome address
3. Overview of available large language model AI tools
4. Subgroup updates[2]
5. Breakout sessions – Subgroups 1 and 3[3]
6. Breakout sessions – Subgroups 2 and 4[4]

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1 A grouping of countries with emerging economies that includes Brazil, the Russian Federation, India, China, South Africa, and other members.

2 While agenda items 4, 5, 6, 14, 15, and 16 were discussed separately during the meeting, they are reported herein under a single agenda item for clarity and to minimise duplication.

3 Ibid.

4 Ibid.

7. Generative AI for drug design and molecular discovery – with a live demonstration
8. The development of AI technology and paradigm shift driven by AI in chemical research
9. The new workflow for science: clash of mathematics, high-performance simulation, and AI
10. AI as a chemical intelligence and forecasting tool
11. Embodied AI technology for high-risk task operations
12. Recent density functional theory and AI-based methods for the identification of novel chemical agents and synthetic drugs
13. Cirrus and the AI Africa Consortium: towards building Africa's largest AI infrastructure and training platform
14. Breakout sessions – Subgroups 1 and 4[5]
15. Breakout sessions – Subgroups 2 and 3[6]
16. Plenary discussion[7]
17. Next steps, closing remarks, any other business
18. Closure of the meeting

2. AGENDA ITEM TWO – Welcome address

2.1 Dr Wu opened the meeting by welcoming the participants before providing a brief overview of how AI is developing both globally, and in China. He highlighted key statistics about development in China, including the value of its AI industry, and the number of research papers published, patent applications filed, and AI companies established. In addition to its initiatives in international AI governance, he described China's national regulatory framework for generative AI, which includes legislation, regulations, and standards.

2.2 Dr Wu outlined four principal areas of AI development in China—large language models, multimodal models, autonomous agents, and embodied intelligence—and described key trends in each. He noted that in 2024, the most advanced AI systems surpassed human performance on challenging benchmarks, including on doctorate-level science questions. He further highlighted that in 2025, Chinese AI models have advanced rapidly and are now achieving progress on a par with cutting-edge international models in foundational capabilities.

2.3 Describing the national AI Capacity-Building Action Plan for Good and for All, Dr Wu described the AI Plus initiative, which aims to empower the economy by applying AI in areas such as industrial manufacturing, agriculture, and climate change response, and to enable the sound development of AI for the greater good. In order to prepare for the full impact of the arrival of the AI era, China is ensuring that four pillars (platform

5 Ibid.
6 Ibid.
7 Ibid.

construction, data governance, operations and maintenance management, and risk control) are being strengthened. Large models are in the early exploration phase in industry and are being considered within the research and development, equipment, production, and management sectors.

2.4 In closing, Dr Wu highlighted the work of CAICT in supporting AI development in China. He noted that in 2017, CAICT and other organisations established the Artificial Intelligence Industry Alliance in China. CAICT is also supporting international partners, including BRICS. Dr Wu noted that BRICS countries recognise the role of AI in global sustainable development and the need for cooperation to benefit society and humanity. Finally, Dr Wu noted that CAICT has been contributing to the AI Readiness Framework that has been developed by the International Telecommunication Union.

3. AGENDA ITEM THREE – Overview of available large language model AI tools

3.1 Dr Michael Kuiper from Google DeepMind, based in the United Kingdom of Great Britain and Northern Ireland, provided an overview of large language models (LLMs) as of June 2025. He introduced the main models available and provided advice on their use.

3.2 These models have evolved from chatbots and are trained on large datasets from which they learn the association between words, helping them to build general knowledge about the world. Increasingly, LLMs are becoming multimodal and running programs or solving tasks jointly with other LLMs. Over time, prices have become more competitive, and the number of models to choose from has increased, while previous issues with hallucination (producing faulty output) have decreased.

3.3 Since the launch of ChatGPT by OpenAI in November 2022, which first brought broader attention to LLMs and AI, other companies have released models including Claude (Anthropic), DeepSeek (DeepSeek), Gemini (Google DeepMind), and Llama (Meta). Dr Kuiper explained that different models have different strengths, excelling at mathematics or performing better in "deep research" mode, which facilitates compiling comprehensive reports on a topic. To compare models, open leaderboards (for example, from Vellum AI) can be accessed, supporting decision-making in selecting the most appropriate AI tool for a given task. Dr Kuiper highlighted that Llama and DeepSeek are open models and can be downloaded for offline use. Besides the main models, AI research tools, such as Perplexity, Elicit, or NotebookLM, enable the generation of a synopsis while providing references.

3.4 Advising on how to make the most out of AI tools, Dr Kuiper emphasised keeping up to date, as the field is developing rapidly. He additionally recommended keeping data security in mind, double-checking source material in responses, and using each model according to its strengths. Concluding his presentation, he expressed caution when using AI for tasks and advocated for a "think first, AI augment later" strategy.

3.5 In the discussion that ensued, the limitations and challenges of LLMs were addressed. With increasing AI-generated content, the consequences of LLMs being trained on LLM-generated data were discussed. In this context, the importance of having a human in the loop was emphasised. Further comments underscored that output from LLMs is inherently probabilistic—answers will never be 100% accurate.

4. AGENDA ITEMS FOUR, FIVE, SIX, FOURTEEN, FIFTEEN, AND SIXTEEN – Discussion on subgroup topics

4.1 Subgroup 1, led by Dr Kuiper, is focused on synthesis and retrosynthesis prediction, as well as the automated and remote production of chemicals. During its discussions, the subgroup examined the dual-use implications of AI-enabled retrosynthesis platforms and chemical structure generation tools, recognising these technologies as inherently dual-use while identifying specific practical opportunities and threats.

4.2 When chemical structures of concern are known, Subgroup 1 noted that retrosynthesis tools provide significant value to chemical security and regulatory agencies. Current technologies enable analysts to map feasible synthetic pathways to target compounds, potentially uncovering routes using unregulated precursors or non-obvious starting materials. These insights can broaden knowledge prior to OPCW inspections and also support research efforts in OPCW designated laboratories and other regulated environments. Modern platforms incorporating scalability data and optimal reaction conditions could allow regulators to focus on routes suitable for scale-up operations.

4.3 Subgroup 1 identified a limitation: retrosynthetic analysis effectiveness depends on detailed knowledge of target molecule structures. When threat identities are unknown, retrosynthesis software cannot generate meaningful insights. While forward synthesis prediction and AI-based chemical generators can propose derivatives of known agents, they typically produce large, nebulous structure sets that make threat prediction and prioritisation extremely difficult given limited resources and complex experimental identification requirements.

4.4 In its review of publicly available tools, including ASKCOS, IBM RXN, and AiZynthFinder, Subgroup 1 determined that, while accessible, these data-driven platforms typically point users towards established synthetic routes published in the scientific literature. Discovering new pathways, in particular to synthesise complex or novel molecules (such as natural products with complex chemical structures), requires more sophisticated platforms capable of creative chemical reasoning. Importantly, qualifying AI-generated novel routes still requires deep human expertise to assess feasibility, making human oversight essential rather than optional.

4.5 Discussions highlighted how AI now facilitates the generation of chemical structures with novel atom connectivities not yet in public databases. Despite the large number of known compounds, the theoretical space for novel molecules remains astronomically vast. AI also aids in predicting molecular properties, which are particularly important in drug discovery where balancing desired biological effects against toxicity and side effects remains challenging. This capability extends beyond pharmaceuticals to potential dual-use applications.

4.6 Subgroup 1 identified a critical bottleneck: While AI effectively generates novel structures in silico with potentially desirable and user pre-defined properties, experimental testing is still essential to confirm these properties. This gap between computational prediction and experimental testing represents both a current limitation and a potential monitoring control point.

4.7 Both open-source and commercial molecular design tools rely heavily on public or proprietary databases, creating dependencies affecting capability and accessibility. The subgroup noted ongoing challenges in the quality and reliability of the information (for example, data curation protocols), plus storing and sharing large chemical libraries, with implications for both legitimate research and potential misuse monitoring.

4.8 Subgroup 1 concluded that retrosynthesis software offers powerful capabilities for both chemical research and security applications. However, its effectiveness in monitoring and prevention depends critically on having actionable intelligence about specific compounds of concern, emphasising the continued importance of traditional threat assessment methodologies alongside these emerging AI capabilities.

4.9 Subgroup 2, led by Dr Roy Forbes, is focusing on data curation, protection, and reliability. During the intersessional period, the subgroup developed a series of tables that will be populated and will assist subgroup members in presenting their findings and providing recommendations.

4.10 In terms of data curation, Subgroup 2 is considering how information may be organised, extracted, and contextualised for monitoring and verification purposes. For data protection, Subgroup 2 is exploring methods to secure sensitive data, ensure access controls, and prevent data tampering or manipulation. Finally, regarding data reliability, the subgroup is considering how to ensure data accuracy, verifiability, explainability, and trustworthiness in high stakes assessments. In each of these areas, Subgroup 2 is compiling potential actions and formulating recommendations that relate to assessing new capabilities, mapping current limitations and persistent challenges, and identifying external non-technical influences. These actions and recommendations were discussed at length during the meeting.

4.11 Subgroup 2 is also reviewing the work in this space being conducted by similar organisations, namely the International Atomic Energy Agency (IAEA), the World Health Organization (WHO), the Implementation Support Unit of the Biological Weapons Convention, the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO), the International Criminal Police Organization (INTERPOL), and Europol. In its review, the subgroup sought to identify aspects of work of these organisations that could be relevant to the OPCW. These include data authentication and security, data sharing protocols, data governance frameworks, leveraging intelligence from open sources, and AI-driven sensor networks. Subgroup 2 also discussed key lessons that could be considered by the OPCW.

4.12 Subgroup 3, led by Prof. Keunhong Jeong, continued its examination of the intersection between AI and the implementation of the Chemical Weapons Convention (the Convention), with particular focus on verification capabilities, dual-use risks, and governance strategies. During the second meeting of the TWG, Subgroup 3 advanced its discussions on areas 6(d) and 6(e) of the terms of reference of the TWG[8] and refined its work across three interconnected themes: AI-enhanced chemical analysis and verification; opportunities and risks of new AI capabilities; and governance mechanisms and capacity building for AI in chemical security.

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[8] The complete terms of reference for the TWG on AI are provided in Annex 1 to SAB-40/WP.1 (dated 11 April 2025).

4.13 Regarding AI-enhanced chemical analysis and verification, Subgroup 3 examined recent progress in the capacity of AI to predict physico-chemical and toxicological properties with high accuracy, particularly through transformer-based models and graphing neural networks. These developments support improved chemical identification and verification processes, notably in spectral analysis (including mass spectrometry, infrared spectroscopy, and nuclear magnetic resonance (NMR) spectroscopy), where AI integration significantly reduces interpretation time while increasing precision.

4.14 In addition, Subgroup 3 discussed how AI-powered sensor fusion can synthesise data from several modalities, including hyperspectral imaging and acoustic sensors, leading to near real-time threat detection with improved accuracy. New tools also enable field-deployable systems with edge computing capabilities. However, the subgroup acknowledged the ongoing need for human oversight, particularly to verify AI-generated outputs and mitigate the risks of false predictions.

4.15 In terms of opportunities and risks, Subgroup 3 identified several novel AI applications in chemical threat detection and mitigation. These included:

(a) AI-assisted remote sensing, combining satellite, drone, and ground sensor data to detect chemical activities;

(b) predictive analytics using open-source information to anticipate emerging threats; and

(c) AI-driven rapid discovery of medical countermeasures, compressing development timelines to a fraction of traditional efforts.

4.16 Conversely, Subgroup 3 members underscored heightened dual-use concerns, including the accessibility of generative AI tools that can support synthesis route planning for illicit chemicals, and the susceptibility of AI models to adversarial manipulation, data poisoning, and deepfake generation. These trends call for urgent attention to AI misuse prevention within the framework of the Convention.

4.17 To address the above challenges, Subgroup 3 proposed a suite of potential governance and capacity-building measures. These could include the creation of a permanent AI Unit under the SAB, the development of AI ethical guidelines tailored to the chemical security domain, and the establishment of monitoring systems for dual-use AI applications within the OPCW.

4.18 Subgroup 3 also reviewed global governance models—including the European Union AI Act, the National Institute of Standards and Technology (NIST) AI Risk Assessment Framework, and the International Organization for Standardization/International Electrotechnical Commission (ISO/IEC) 42001 Standard—as potential references for OPCW engagement. Proposals for international cooperation included forming an AI–Chemical Weapons Convention implementation consortium and enhancing OPCW partnerships with other international organisations such as the United Nations, the WHO, and the IAEA.

4.19 Subgroup 4, led by Col. Povoden, is examining AI-supported simulation and training tools. During its discussions, the subgroup focused on identifying existing state-of-the-art technologies in this area, while considering potential future applications and addressing gaps, specifically within the context of meeting OPCW training needs.

4.20 Subgroup 4 continued its discussions on various extended reality tools. It noted that these tools benefit from the integration of AI, resulting in realistic sensor data and dynamic scenarios and set-ups. It was considered that the inclusion of chemical dispersion models will also be possible in the near future. Subgroup members agreed that selecting the most appropriate tools for training requires specific knowledge and insights into the skill level within an organisation. To this end, they proposed that the OPCW should consider employing a suitably qualified and experienced staff member, such as a data scientist, who would be responsible for this task.

4.21 The subgroup noted the existence of AI-supported training tools designed for military applications (for example, simulating high-threat scenarios in both rural and urban environments), as well as for civilian use in first response to chemical incidents and in medical training for chemical exposure. The subgroup considered that these tools could be adapted to the needs of the OPCW.

4.22 Subgroup 4 also considered data protection and ethical aspects, as various personal data are collected using such tools. When online or cloud-based applications are used, there is a risk that information and gaps may be exposed. The subgroup agreed that it is better to use stand-alone, offline AI-supported tools for realistic training activities. Furthermore, for ethical reasons, it was proposed that the visual portrayal of casualties should not be too realistic.

4.23 Finally, the advantages, challenges, and limitations of AI-supported training tools were discussed. Subgroup 4 noted that such tools offer a low-cost opportunity to simulate complex environments and are easy to repeat with flexible applications, which are significant advantages. A downside is that virtual reality (VR) goggles may cause cyber sickness, resulting in headaches, nausea, and disorientation. Ensuring that scenarios are as realistic as possible remains a challenge. Despite the challenges and limitations, improvements continue to be made in this area and recently, VR goggles have been successfully integrated with a respirator and demonstrated at the OPCW.

4.24 Testing of currently available systems indicates that the most effective use of these tools is through a hybrid approach. AI can effectively support the creation and visualisation of realistic scenarios, planning processes, equipment and asset selection, and the consideration of safety and security aspects. The subgroup agreed that any implemented VR training sessions should be interspersed with practical tasks—such as sampling, donning, doffing, and note-taking—as these activities require hands-on practice in real-world conditions.

5. AGENDA ITEM FIVE – Breakout sessions – Subgroups 1 and 3

See agenda item 4.

6. AGENDA ITEM SIX – Breakout sessions – Subgroups 2 and 4

See agenda item 4.

7. AGENDA ITEM SEVEN – Generative AI for drug design and molecular discovery – with a live demonstration

7.1 Prof. Hajar Mousannif and Dr Mohamed Amine Chadi from the Cadi Ayyad University, Morocco, presented their research on the use of generative AI for molecular discovery and drug design. Besides the potential of generative AI to accelerate conventional drug design, the speakers emphasised the risk of misuse, outlining how their work can help in increasing dual-use awareness and facilitate discussions about the ethical use of AI in chemistry.

7.2 Before exploring AI-based molecular discovery, Prof. Mousannif provided an overview of AI and its subfields. With AI as the umbrella term, the field is structured into machine learning and deep learning, with the latter describing a certain type of machine learning algorithms. At its core, machine learning algorithms are designed to learn patterns from data, relying on a representation component (for example, a neural network), an evaluation component, and an optimisation component. However, learning strategies can differ, leading to three machine learning families: supervised learning, unsupervised learning, and reinforcement learning.

7.3 Supervised learning relies on labelled data and can perform regression (for example, linking salary to work experience) and classification tasks, such as determining the probability of diabetes considering age, weight, or body mass index. Unsupervised models learn from unlabelled data. The applied algorithms excel in clustering data points based on similarity and reduce complexity through dimensionality reduction. Reinforcement learning is powerful in decision-making. An agent trained through reinforcement learning receives reward feedback for actions, thereby iteratively improving decision-making. This results in agents capable of making complex decisions, such as predicting the best move in a game of "Go".

7.4 For drug design and molecular discovery, reinforcement learning is often applied. Using simplified molecular input line entry system (SMILES) notation, a string-based representation of molecules[9]—which includes information about their composition and structures—any language model (such as ChatGPT) can be used to generate novel molecules. To produce desirable molecules based on parameters or objectives (for example, target binding characteristics), the language model—also known as the generative model—is coupled to the predictive (evaluation) model. Over many iterations, the feedback provided by the predictive model will prompt (reinforce) the generative model to produce desirable molecules.

7.5 In their research, Prof. Mousannif and colleagues have developed a novel approach to reinforcement learning, which has been termed "conditional reduction of the loss value (CRLV)". Benchmarking the CRLV approach to the current state-of-the-art approach showed that using CRLV generated more desirable molecules, based on a pre-determined set of objectives.

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9 Popova, Mariya, Olexandr Isayev, and Alexander Tropsha. "Deep Reinforcement Learning for de Novo Drug Design." *Science Advances* 4, no. 7 (July 6, 2018). https://doi.org/10.1126/sciadv.aap7885.

7.6 Dr Chadi concluded the presentation with a live demonstration of Molecure.ai, a generative AI-based molecular design platform developed by the speakers. He demonstrated that the tool can be used to generate novel molecules by selecting desired objectives and choosing between different AI models.

7.7 The presentation elicited multiple questions from the audience. Regarding Molecure.ai, participants enquired about including more specific properties (such as protein binding) when generating compounds, integrating other models in the platform, and comparing generated compounds against pre-existing databases. Addressing reinforcement learning and AI-based molecular discovery, questions were raised regarding the non-uniqueness of SMILES, the need for graphical representation, and the synthetic accessibility of generated molecules.

8. AGENDA ITEM EIGHT – The development of AI technology and paradigm shift driven by AI in chemical research

8.1 Dr Ning Xia from Chemical.AI, based in China, examined the impact of AI on chemical research, especially highlighting the novel approaches AI brings to synthesis route design and laboratory automation. He also considered the risks and opportunities of AI in chemistry.

8.2 Digitalisation of chemistry is driven by AI-based technologies, impacting multiple areas such as chemical biology, digital medicine, data analysis, material science, simulation and modelling, supply chains, laboratory and process innovations, and environmental technologies. Dr Xia highlighted examples of AI advancing molecular synthesis and drug discovery by accelerating the identification of potential drug candidates. In materials science, a recently published study showed the creation of 41 novel inorganic compounds within 17 days, utilising an AI-driven platform.[10] Furthermore, automated, AI-guided laboratories allow for higher precision and reproducibility, real-time data collection and analysis, smart control of chemical processes, and high-throughput experimentation.[11]

8.3 In synthesis route design, AI can be applied to retrosynthesis. Retrosynthesis provides insights into potential synthesis routes by analysing how to break a target molecule into commercially available starting materials. Elaborating on the use of AI in retrosynthesis, Dr Xia presented a hybrid model approach that combines rule-based expert systems (relying on retrosynthesis templates based on chemical reactions) and data-driven deep learning models. Complementing the approach with reaction condition search tools allows for assessing the risk and feasibility of a reaction within a route, while additionally optimising conditions to improve yield. Dr Xia commented that AI-based retrosynthesis software can perform well for up to 10 synthesis steps but still struggles with longer, more complex synthesis. Additionally, AI tools can be applied to forward synthesis. In forward synthesis, a chemical route is built from the starting material, leading to one or multiple target molecules. In this way, AI can be used to generate synthesisable virtual molecular libraries, streamlining drug design.

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10 Merchant, Amil, Simon Batzner, Samuel S. Schoenholz, Muratahan Aykol, Gowoon Cheon, and Ekin Dogus Cubuk. "Scaling Deep Learning for Materials Discovery." *Nature* 624, no. 7990 (November 29, 2023): 80–85. https://doi.org/10.1038/s41586-023-06735-9.

11 Szymanski, Nathan J., Bernardus Rendy, Yuxing Fei, Rishi E. Kumar, Tanjin He, David Milsted, Matthew J. McDermott, et al. "An Autonomous Laboratory for the Accelerated Synthesis of Novel Materials." *Nature* 624, no. 7990 (November 29, 2023): 86–91. https://doi.org/10.1038/s41586-023-06734-w.

8.4 Touching on the interplay between AI and laboratory automation, Dr Xia briefly illustrated that automated systems are often composed of different modules, such as a reaction module or a purification module. He highlighted that in specific examples, automation leads to a 20- to 40-fold increase in efficiency when compared to traditional manual labour.

8.5 Dr Xia noted that in terms of preventing the re-emergence of chemical weapons, AI brings both tangible risks and opportunities. LLMs enable easier access to information, and AI-guided synthesis route design will provide a magnitude of ways to produce chemical weapons, making regulatory control of starting materials more challenging. Highlighting the risks, Dr Xia showed that Chemical.AI's ChemAIRS software could generate 10 synthesis routes for sarin and VX and provide 30 similar molecules in just 30 seconds. Conversely, AI-based molecular design tools can be used to pre-emptively ban dangerous molecules or extend the monitoring of starting materials. AI can thereby facilitate the establishment of preventive regulation, adapting to the risks resulting from its use in chemistry.

8.6 TWG members posed questions on the current state of the art of AI in chemical research. They also discussed the challenges faced when applying AI-based retrosynthesis to complex molecules with multiple stereocentres, the current restrictions of synthesis automation in multistep synthesis routes, and reaction scales carried out by automated systems. Furthermore, questions were raised about the ChemAIRS prediction software, enquiring about impurity, catalyst, solvent, and reaction success prediction. Additionally, the regulation of automation and starting materials was discussed, as was the blacklisting of compounds in AI tools.

9. AGENDA ITEM NINE – The new workflow for science: clash of mathematics, high-performance simulation, and AI

9.1 Prof. Simon See from the NVIDIA AI Technology Center, Singapore, gave an overview of his research on the intersection of mathematics, high-performance simulation, and AI. His domain of studies includes category theory, the mathematical foundations of AI, and its application in various scientific domains such as climate science, life sciences, and healthcare.

9.2 Prof. See began his presentation by explaining the basic mathematical concepts underlying AI and the different types of modelling used by current AI agents. He then outlined the objectives of his research team, which include providing AI assistance to scientific researchers and pursuing "fully automated open-ended scientific discovery". He emphasised the importance of assistance domain adaptation for achieving this goal, describing it as a model's ability to transfer knowledge from one discipline to another using acquired data.

9.3 Prof. See also presented the latest advances in natural language processing and its applications in various fields, including the development of AI agents capable of performing complex tasks autonomously.

9.4 Prof. See highlighted the integration of physics and neural networks,[12] specifically through physics-informed neural networks and neural operators. He explained how these techniques are revolutionising the way differential equations are solved, combining the strengths of neural networks with physics-based models to achieve more accurate and efficient solutions. Throughout the presentation, TWG members commented on the fundamentals of mathematical modelling, the objectives of his team, and the future of AI-based emerging technologies. Prof. See noted that definitive conclusions in this area remained challenging and emphasised both the ongoing nature of their research and the field.

9.5 Prof. See concluded his presentation by discussing the future directions of AI research and its potential to revolutionise various industries. He underscored the importance of a technology regulation body that can provide educated legislative recommendations, given the rapid pace of technological progress in the field of AI.

10. AGENDA ITEM TEN – AI as a chemical intelligence and forecasting tool

10.1 Prof. Bartosz Grzybowski, representing both the Polish Academy of Sciences and the Ulsan National Institute of Science and Technology in the Republic of Korea, focused on how data-driven forecasting in chemistry may be used both to benefit humankind—through the development of life-saving drugs, for example—and to cause intentional harm, through the production of hazardous chemicals.

10.2 For computers to be effective in helping chemists solve complex synthesis issues such as the production of pharmaceuticals, they need to learn the rules and constraints of chemistry (including the movement of electrons, chirality, and stereochemistry). Prof. Grzybowski explained that AI systems have learned how to play and win games of chess, as there are fewer than 15 possible moves with well-defined applicability. Conversely, successful organic synthesis using AI is more challenging as these "moves" (in other words, the types of chemical reactions) exceed 100,000, and their applicability is contextual and dependent on the specific molecules involved. AI cannot learn the rules of synthesis simply by accessing every chemical publication available, as they will only indicate successful reactions and do not generally provide information on unsuccessful and unproductive reactions, which is critical to this learning process.

10.3 To overcome this limitation, the Grzybowski research group has developed hybrid models that leverage a combination of AI, quantum mechanics, and molecular mechanics, affording the system a greater understanding of the rules of chemistry and leading to viable synthetic plans. In 2017, one of the research group's advanced algorithms, Chematica,[13] was used to generate synthesis routes for several challenging drug compounds, which were subsequently validated experimentally. Prof. Grzybowski underscored the fact that experimental validation of AI outputs in chemistry is essential. Since then, their algorithms have been used to synthesise a number of complex natural products, including cephanolide B and scabrolide A.

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12 Raissi, Maziar, Paris Perdikaris, and George Em Karniadakis. "Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations." *Journal of Computational Physics* 378 (February 2019): 686–707. https://doi.org/10.1016/j.jcp.2018.10.045.

13 Grzybowski, Bartosz A., Sara Szymkuć, Ewa P. Gajewska, Karol Molga, Piotr Dittwald, Agnieszka Wołos, and Tomasz Klucznik. "Chematica: A Story of Computer Code That Started to Think like a Chemist." *Chem* 4, no. 3 (March 2018): 390–98. https://doi.org/10.1016/j.chempr.2018.02.024.

10.4 Prof. Grzybowski then addressed challenges that extend beyond academia, including issues of scale, supply chains, forecasting, and threat anticipation. For AI-designed chemical synthesis to be viable in industrial settings, computers must not only generate synthetic pathways, but also factor in production costs. This involves decisions such as whether to incorporate inexpensive materials early or later in the process, whether to pursue linear or convergent pathways, and—if using convergent synthesis—where the optimal point of convergence should be. To evaluate these variables, Prof. Grzybowski introduced a recursive up-propagation formula to estimate reaction costs. He also presented a method to classify reactions by scale—laboratory (grams), pilot (kilograms), and industrial (tonnes)—and demonstrated how this classification can be used to assess the total cost of a synthetic process.

10.5 Demonstrating Allchemy,[14] a newer generation platform developed in his research group, Prof. Grzybowski explored how supply chains could be re-routed in response to feedstock shortages. Using paracetamol production and recent geopolitical market disruptions as an example, he demonstrated supply chain optimisation through a comprehensive plan to map the production pathways of the most essential medicines in the United States of America, aiming to identify as many shared intermediates as possible. As a further example, he demonstrated how the production of the top 51 medicines in the United States could be fine-tuned by identifying overlapping intermediates. The number of required compounds was reduced from 626 to 404, streamlining the overall production process. He also noted that the Allchemy platform can be leveraged to identify how waste chemicals can be used to generate valuable ones, such as pharmaceuticals. Approximately 300 different pharmaceuticals can be produced from this waste, including a drug to treat leprosy that can be produced from plastic bottles and phenol from coal production.[15] These examples illustrate the potential for creating a circular chemistry model that promotes sustainability and resource efficiency.

10.6 Lastly, Prof. Grzybowski described some of the harmful substances whose production may be facilitated by AI. He noted that in just 15 minutes, an algorithm discovered all possible ways to synthesise fentanyl, involving a total of approximately 350 different chemicals. Of these, only 13 are subject to regulation in the United States of America. The chemical drug problem also arises when existing cannabinoid derivatives are banned, with new derivatives being predicted by computer programs and appearing shortly afterwards. Prof. Grzybowski then explained how to identify potential fentanyl analogues ranked by the predicted μ-opioid receptor binding potency. The same algorithm was used to generate possible analogues of the so-called "novichok" chemicals. In closing, Prof. Grzybowski discussed how AI systems incorporating an advanced level of chemistry could also be used to predict the degradation of chemical warfare agents.

10.7 Prof. Grzybowski concluded by underlining the duality of chemical AI, the seriousness of its development in modelling entire networks of chemical industries, and its power in monitoring, anticipating, and curtailing the production of harmful agents. Questions from TWG members touched on such topics as knowledge accumulation and AI applicability, privacy and fairness, the need for monitoring of chemical production, and difficulties related to data management and the data transparency of chemical companies.

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14 https://allchemy.net/.

15 Wołos, Agnieszka, Dominik Koszelewski, Rafał Roszak, Sara Szymkuć, Martyna Moskal, Ryszard Ostaszewski, Brenden T. Herrera, et al. "Computer-Designed Repurposing of Chemical Wastes into Drugs." *Nature* 604, no. 7907 (April 27, 2022): 668–76. https://doi.org/10.1038/s41586-022-04503-9.

11. AGENDA ITEM ELEVEN – Embodied AI technology for high-risk task operations

11.1 Prof. Bin Fang from the Beijing University of Posts and Telecommunications, China, presented his research on embodied AI technology. Focusing on tactile sensing and the integration of LLMs into robotics, Prof. Fang highlighted that these technologies enable high-risk task operations.

11.2 Confronted with potential threats, chemical or otherwise, robots with AI integration can be crucial for emergency responses and support hazard detection, rescue operations, or explosive handling. To be effective at these high-risk tasks, sensory systems—especially tactile sensing—are often crucial. Prof. Fang's research centres around vision-based tactile sensors that utilise high-resolution optical measurements to capture deformations on a contact medium, leading to higher information density compared to electronic tactile sensors.[16] Structurally, vision-based tactile sensors are composed of a contact module, camera module, and illumination module.[17]

11.3 Over the past five years, vision-based tactile sensors have moved into a miniaturisation and integration stage; however, challenges remain in aspects such as durability, sensitivity, or capturing multiple types of tactile information (multimodal). As part of his team's work on hardware development, Prof. Fang presented their advances in process formulation and coating preparation. Their novel coating process has resulted in micron-level tactile spatial resolution and increased wear resistance. In addition, he highlighted the development of a multimodal sensor, capable of capturing both visual and tactile information, thereby increasing sensory information input for robotic systems deployed in high-risk emergency scenarios.

11.4 Building and testing each sensor variation can be time consuming, which led Prof. Fang and his team to develop the Tacchi series contact simulator, in which testing can be performed before transferring the gathered knowledge to real-world applications (so-called "sim-to-real transfer"). Simulations were used to evaluate RobotGPT, a decision-making framework for robotic manipulation trained with ChatGPT, which illustrates how foundation models can be embedded into manipulation tasks.[18] RobotGPT first learned in simulation, and then was deployed in the real world.

11.5 The presentation prompted a fundamental discussion among the participants about the efforts in robotics to mimic humans. Questions were raised about the research effort spent on mimicking humans versus developing novel sensing modalities beyond human capabilities. In response, it was argued that mimicking humans already provides formidable challenges, that human creative bias might be involved, and that robots would be part of a world designed by and for humans.

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16 Lepora, Nathan F. "The Future Lies in a Pair of Tactile Hands." Science Robotics 9, no. 91 (June 26, 2024). https://doi.org/10.1126/scirobotics.adq1501.

17 Bauza, Maria, Antonia Bronars, Yifan Hou, Ian Taylor, Nikhil Chavan-Dafle, and Alberto Rodriguez. "SimPLE, a Visuotactile Method Learned in Simulation to Precisely Pick, Localize, Regrasp, and Place Objects." *Science Robotics* 9, no. 91 (June 26, 2024). https://doi.org/10.1126/scirobotics.adi8808.

18 Jin, Yixiang, Dingzhe Li, Yong A, Jun Shi, Peng Hao, Fuchun Sun, Jianwei Zhang, and Bin Fang. "RobotGPT: Robot Manipulation Learning from ChatGPT." *IEEE Robotics and Automation Letters* 9, no. 3 (March 2024): 2543–50. https://doi.org/10.1109/lra.2024.3357432.

12. AGENDA ITEM TWELVE – Recent density functional theory and AI-based methods for the identification of novel chemical agents and synthetic drugs

12.1 Prof. Jeong from the Korea Military Academy, Republic of Korea, discussed the significant advances and challenges in the field of chemical research and development, particularly focusing on the integration of AI and density functional theory (DFT) in identifying new chemical agents and synthetic drugs.

12.2 Prof. Jeong began by highlighting the transformative role of AI in chemical research and development. He explained that AI accelerates the discovery of new materials, enhances protein structure prediction capabilities through tools like AlphaFold, and optimises chemical processes and reactions. However, these advances could also lead to the design of new toxic chemicals at a lower cost that require smaller facilities.

12.3 However, the integration of AI in chemical research presents several challenges. Prof. Jeong noted the difficulties in analysing unknown toxic substances and the lack of threat profiles for novel synthetic compounds. He underscored the importance of managing false positives and false negatives in AI detection systems, and the potential misuse of AI technologies in chemical weapons development.

12.4 To address these challenges, Prof. Jeong proposed the development of AI-based chemical detection technologies. He suggested that AI could predict the chemical and physical threat profiles of substances and develop standardised AI-based inspection tools. He also stressed the need for international cooperation and ethical guidelines to prevent the misuse of AI in chemical weapons development. Prof. Jeong's overall recommendation was to acknowledge the imminent reality of the impact of AI on chemical security and to leverage associated new technology to enhance implementation of the Convention; this would require immediate action, international cooperation, and continued innovation, leading to a new era in chemical security.

12.5 Prof. Jeong then presented AI-based chemical detection technologies in more detail. He discussed the use of quantum chemical calculations[19,20] and spectroscopy integrated identification methods[21] for analysing unknown chemicals. These methods incorporate experimental and theoretical data from various spectroscopic techniques in order to provide accurate identification of unknown substances.

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19 Kim, Hee-Kyung, Hyejin Cho, Keunhong Jeong, Ung Hwi Yoon, and Hye-Ryun Cho. "Thermodynamic Study of Am(III)–Isosaccharinate Complexation at Various Temperatures Implicating a Stepwise Reduction in Binding Denticity." *Inorganic Chemistry* 61, no. 48 (November 23, 2022): 19369–78. https://doi.org/10.1021/acs.inorgchem.2c03180.

20 Kim, Hee-Kyung, Keunhong Jeong, Hye-Ryun Cho, Kyungwon Kwak, Euo Chang Jung, and Wansik Cha. "Study of Aqueous Am(III)-Aliphatic Dicarboxylate Complexes: Coordination Mode-Dependent Optical Property and Stability Changes." *Inorganic Chemistry* 59, no. 19 (September 18, 2020): 13912–22. https://doi.org/10.1021/acs.inorgchem.0c01538.

21 Jeong, Keunhong, Honghyun Kim, Sein Min, Young Wook Yoon, Yoonjae Cho, Choon Hwa Park, Tae In Ryu, Seung-Ryul Hwang, and Sung Keon Namgoong. "DFT–Spectroscopy Integrated Identification Method on Unknown Terrorist Chemical Mixtures by Incorporating Experimental and Theoretical GC-MS, NMR, IR, and DFT-NMR/IR Data." *Analytical Chemistry* 96, no. 2 (December 28, 2023): 694–700. https://doi.org/10.1021/acs.analchem.3c03647.

12.6 Prof. Jeong also highlighted the importance of building reliable databases without synthesis, using quantum chemical calculations to predict spectra of unknown materials. This approach, he explained, could significantly enhance the accuracy and efficiency of chemical identification processes.

12.7 In the latter part of his presentation, Prof. Jeong discussed the potential of quantum sensing and AI in detecting low-concentration chemicals. He explained that quantum hyperpolarisation techniques could enhance the signal-to-noise ratio in NMR, making it possible to detect chemicals at much lower concentrations than traditional methods. This advance, he noted, could be particularly useful in detecting chemical weapons and other hazardous substances.

12.8 Prof. Jeong concluded his presentation by emphasising the need for ongoing innovation and international cooperation in the field of chemical research and development. He called for immediate action to leverage AI and quantum technologies to enhance the implementation of the Convention and improve chemical threat defence.

12.9 In the discussion that followed, TWG members raised questions on quantum mechanics and its accuracy, and spectroscopic structural predictions of unknown molecules. Regarding the accuracy of quantum chemical calculations, Prof. Jeong highlighted the use of various approximation methods and new quantum computing algorithms. He noted that spectroscopic structural predictions would rely on databases of known property data.

13. AGENDA ITEM THIRTEEN – Cirrus and the AI Africa Consortium: towards building Africa's largest AI infrastructure and training platform

13.1 Dr Forbes from the University of the Witwatersrand, South Africa, presented his research activities in chemical catalysis, materials science, and AI capacity building in sub-Saharan Africa. He ascribed the lag of the region's adoption of new technologies to resource constraints and structural challenges in the academic system.

13.2 Dr Forbes began his presentation by outlining the materials studied by his research team, their diverse applications, and the possibility of using AI to support the overall research workflow. Dr Forbes emphasised that the main objective of the team was not to develop AI tools, but to utilise existing technologies to optimise laboratory activities and data interpretation. He further explored the necessities of advanced characterisation methods in materials science to study atomic scale structure and how it relates to the structure–property relationship in functional materials. He then noted that Africa lacked advanced research tools such as a synchrotron—a particle accelerator that produces high-intensity electromagnetic radiation—which is an important tool for scientific study and discovery.

13.3 Dr Forbes introduced the AI Africa Consortium, an institution aimed at fostering AI and computational capacity in Africa. It intends to provide open access to computing resources for the academic research industry, while also focusing on training, upskilling, and helping in leveraging AI for local researchers. Dr Forbes described his research team's upcoming collaboration with start-up initiative project, Cirrus, which aims to develop an open-access forum designed to consolidate AI research and application capabilities.

13.4 To advance the traditional technological developments in Africa, Dr Forbes outlined the potential of adopting AI to accelerate the developmental stages of traditional processes of research. However, barriers such as limited infrastructure and network access were also addressed.

13.5 During the discussion, TWG members commented on the role of AI in developing regions, challenges in education, infrastructure, and emigration of skilled professionals—so-called "brain drain". Dr Forbes also highlighted the need for interventions to maintain academic standards and ensure a deeper understanding of the AI-augmented educational environment.

14. AGENDA ITEM FOURTEEN – Subgroups 1 and 4

See agenda item 4.

15. AGENDA ITEM FIFTEEN – Subgroups 2 and 3

See agenda item 4.

16. AGENDA ITEM SIXTEEN – Plenary discussion

See agenda item 4.

17. AGENDA ITEM SEVENTEEN – Next steps, closing remarks, and any other business

The TWG Chairperson and Vice-Chairperson commended the members on a very productive meeting and invited them to work on their respective questions and meet virtually during the intersessional period. They thanked the TWG members and external speakers for their valuable contributions and expressed their appreciation and thanks to Dr Wu for hosting this meeting at the CAICT/BRICS AI Center. The Chairperson noted that the third and final planned in-person meeting of the TWG is scheduled to take place from 16 to 18 September at the OPCW Centre for Chemistry and Technology. No additional points were raised.

18. AGENDA ITEM EIGHTEEN – Closure of the meeting

The Chairperson ended the meeting at 16:54 (China Standard Time) (10:54 (CET)) on 26 June 2025.

ACKNOWLEDGEMENTS

The TWG members thank the guests and members of the Secretariat who participated in discussions. The TWG is very grateful to Dr Wu and his colleagues at CAICT and the BRICS AI Center for hosting and supporting this meeting in China. The TWG also wishes to acknowledge Ms Ernesa Ademagić of the OPCW Office of Strategy and Policy for her support and contributions to the meeting and its preparations. Lastly, the TWG thanks the OPCW Director-General for his establishment and support of the TWG, and acknowledges the generous contributions of the European Union that helps to cover the costs of the Group's work.

Annex: List of Participants at the Second Meeting of the Scientific Advisory Board's Temporary Working Group on Artificial Intelligence

Annex

LIST OF PARTICIPANTS AT THE SECOND MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON ARTIFICIAL INTELLIGENCE

	Participants	**Institution**
1.	Dr Roy Forbes	University of Witwatersrand, South Africa
2.	Prof. Keunhong Jeong*	Korea Military Academy, Republic of Korea
3.	Prof. Anneli Kruve	Stockholm University, Sweden
4.	Dr Michael Kuiper	Google DeepMind, United Kingdom of Great Britain and Northern Ireland
5.	Mr Arthur Li	Chemical.AI, Canada
6.	Prof. José L Medina-Franco	National Autonomous University of Mexico, Mexico
7.	Prof. Hajar Mousannif	Cadi Ayyad University, Morocco
8.	Dr Catharina Müller-Buschbaum*	Accenture, Germany
9.	Col. Günter Povoden	CBRN Defence Centre, Austrian Armed Forces, Austria
10.	Ms Molly Strausbaugh	CAS, United States of America
11.	Dr Tongning Wu	China Academy of Information and Communications Technology, China
12.	Prof. Imee Su Martinez*	University of Philippines Diliman, Philippines
	External Speakers	**Institution**
13.	Dr Mohamed Amine Chadi	Cadi Ayyad University, Morocco
14.	Dr Ning Xia	Chemical.AI, China
15.	Dr Simon See	NVIDIA AI Technology Center, Singapore
16.	Prof. Bartosz Grzybowski*	Ulsan National Institute of Science and Technology, Republic of Korea
17.	Prof. Bin Fang	Beijing University of Posts and Telecommunications, China
	Technical Secretariat Staff	**Division**
18.	Dr Peter Hotchkiss (Secretary to the SAB)	Office of Strategy and Policy

* Member of the SAB.

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