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# CERTIFICATE OF PARTICIPATION

The scientific committee certified that:

## *Mr Hamza Bennacer*

Has presented online Communication, entitled:

« *AI-Powered Prediction of Structural and Electronic Properties of Emerging Semiconductor Materials* ».

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# AI-Powered Prediction of Structural and Electronic Properties of Emerging Semiconductor Materials

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**Abstract:**

The prediction of fundamental physical properties of materials, such as electronic band gap energy and lattice constants, is crucial for accelerating the development of advanced functional materials in energy-related domains like photovoltaics and photocatalysis. Conventional computational methodologies, including density functional theory, often grapple with the trade-offs between computational duration, and predictive accuracy when applied to complex systems such as chalcopyrites and perovskites. To address these issues, this work proposes hybrid artificial intelligence (AI) frameworks that integrate artificial neural networks (ANN), fuzzy logic systems, and advanced metaheuristic optimisation algorithms. For chalcopyrite compounds, we develop an ANN model hybridised with Particle Swarm Optimisation (PSO) to surmount challenges related to local minima entrapment and solution quality, thereby achieving superior convergence and predictive performance for band gap energy of chalcopyrite materials. For simple perovskites $ABC_3$, optimised ANN and PSO-fuzzy logic models are employed to predict lattice constants. Benchmark evaluations using root mean square error, mean absolute error, and the coefficient of determination

demonstrate the robustness and effectiveness of the proposed approaches. The results highlight the potential of AI- and ML-driven predictive models in accelerating the discovery and design of advanced materials with tailored electronic and structural properties.

**Key words:** Lattice constant, band gap, perovskites, chalcopyrites, Machine learning, prediction.