

Quantum-Inspired Tensor Networks for Materials Simulation and AI Applications

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Recent progress in artificial intelligence is creating new opportunities for materials modeling, especially in regimes where conventional numerical methods face severe scaling limits. In this talk, I will present quantum-inspired tensor network methods as efficient and physically structured tools for simulating complex materials, with a focus on representing strongly correlated systems and high-dimensional many-body states in a compact way. I will discuss how tensor-network approaches can be used to study relevant classes of materials and capture physically meaningful correlations while reducing computational cost.

Beyond their use as simulation tools, tensor networks also offer a principled framework for designing and compressing AI models, enabling architectures that are more interpretable, scalable, and physics-aware. This dual role—as engines for materials simulation and as building blocks for advanced AI—suggests a powerful route toward next-generation workflows for materials modeling, prediction, and design.

References

- [1] R Orús - *Annals of physics*, (2014).
- [2] Saeed S. Jahromi, Roman Orus, *Phys. Rev. B* 99, 195105 (2019).
- [3] F Verstraete, V Murg, JI Cirac - *Advances in physics*, (2008).
- [4] Saeed S. Jahromi, Roman Orus, *Scientific Reports* 14, 19017 (2024)
- [5] Andrei Tomut, et. al., *Proceedings of the 33rd European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning (ESANN 2025)*, Bruges, Belgium, pp. 531-537, April 2025. ISBN: 9782875870926