GHENT UNIVERSITY

CENTER FOR MOLECULAR MODELING

VENKAT KAPIL

Assistant Professor at University College London and the London Centre of Nanotechnolgy

Venkat received his undergraduate degree in Theoretical Chemistry from IIT Kanpur in 2015. He earned a PhD in Material Science in Michele Ceriotti's group from the Swiss Federal Institute of Technology Lausanne (EPFL). During his postdoctoral stage at the University of Cambridge, Venkat worked with Angelos Michaelides' research group and others to develop new simulation methods at the intersection of machine learning and quantum statistical mechanics for full quantum first-principles simulations of materials. He received the Swiss National Science Foundation's "Mobility Fellowship," the "Early Career Oppenheimer Fellowship," and the "Sydney Harvey Junior Research Fellowship" from Churchill College, University of Cambridge. Since January 2024, Venkat has joined University College London and the London Centre of Nanotechnology as a Lecturer (Assistant Professor) in the Department of Physics and Astronomy. Venkat Kapil utilizes machine learning-driven techniques to model materials at finite temperatures based on first principles. His research focuses on understanding the thermodynamics, transport, and quantum mechanics of complex nanoscale systems.

will present the lecture entitled

Machine learning for **full** quantum simulations: understanding the behaviours of confined and water

Simulating complex materials, particularly interfacial and confined systems, is challenging due to the interplay of quantum mechanics in both electrons and nuclei. In this talk, I will present recent progress in developing efficient and accurate methods to incorporate these quantum effects. Specifically, I will highlight highly data-efficient approaches for constructing machine learning potentials using only a few tens of reference structures [1] and equivariant models of electronic properties, such as polarization and polarizability tensors, for spectroscopy [2]. Additionally, I will discuss the development of secondary potentials that capture quantum nuclear corrections to Born-Oppenheimer surfaces, enabling approximate quantum dynamics at a classical computational cost [3]. These advancements make full quantum simulations computationally feasible.

As an application of these methods, I will explore the phase behaviour of water confined within nanometer-sized cavities—a model system with implications for water treatment and energy technologies. Using a predictive approach that integrates electronic structure theory, machine learning, and statistical sampling [4], we investigate a water monolayer confined within graphene-like channels. Our findings reveal that monolayer water exhibits rich phase behaviour and is highly sensitive to van der Waals pressure. Beyond ice phases that break traditional ice rules [5], we predict a superionic phase under milder conditions than those required in bulk, with electrical conductivity surpassing that of many battery materials. Notably, quantum nuclear motion significantly lowers the onset of superionic behaviour [6]. Our work demonstrates that nanoconfinement offers a promising avenue for exploiting superionic water at near-ambient conditions.

[1] Kaur, H., Della Pia, F., Batatia, I., Advincula, X. R., Shi, B. X., Lan, J., Csányi, G., Michaelides, A., & Kapil, V. (2024). https://doi.org/10.48550/ARXIV.2405.20217
[2] Kapil, V., Kovács, D. P., Csányi, G., & Michaelides, A. (2023). https://doi.org/10.1039/D3FD00113J
[3] Musil, F., Zaporozhets, I., Noé, F., Clementi, C., & Kapil, V. (2022). https://doi.org/10.1063/5.0120386
[4] Kapil, V., Schran, C., Zen, A., Chen, J., Pickard, C. J., & Michaelides, A. (2022). https://doi.org/10.1038/s41586-022-05036-x
[5] Ravindra, P., Advincula, X. R., Schran, C., Michaelides, A., & Kapil, V. (2024). https://doi.org/10.1038/s41467-024-51124-z
[6] Ravindra, P., Advincula, X. R., Shi, B. X., Coles, S. W., Michaelides, A., & Kapil, V. (2024). https://doi.org/10.48550/ARXIV.2410.03272

WHEN? Tuesday December 17, 2024 at 14h00

WHERE? Class room 2.3 (former industrieel beheer), 2nd floor
Tech Lane Ghent Science Park, Campus Ardoyen
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