CHEMISTRY & CHEMICAL BIOLOGY COLLOQUIUM: Entropic and Quantum Effects at Solid/Liquid Interfaces

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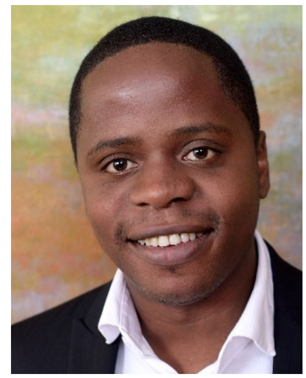
Date:
3/5/2021

Time:
2:30 PM-4:00 PM

Link:
Please contact snsgradstaff@ucmerced.edu for the Zoom link and passcode.

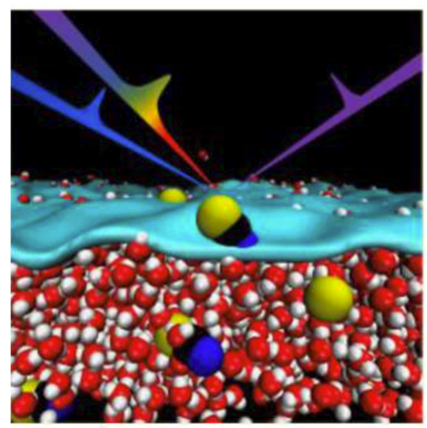
About The Speaker:



Tod Pascal is the PI of the ATLAS Materials Physics Lab at UCSD, whose research lies at the intersection of computer science, chemical physics, spectroscopy and statistical thermodynamics. Research projects utilize computational and theoritical tools to elucidate the properties of nanoscale materials, with particular focus on energy storage and catalysis. He is the co-lead of an integrated research group in the UCSD MRSEC, focused on predictive assembly. He is also a PI in the Sustainable Power and Energy Center, the Institute for Materials Design and Discovery and the Halıcıoğlu Data Science Institute at UCSD. He received his PhD in Chemistry at Caltech working with Bill Goddard, was an NSF International Postdoctoral Fellow at KAIST, Korea and later a DOE Postdoctoral fellow at LBNL.

Abstract:

The thermodynamic stability of water next to graphitic surfaces is of fundamental interest, as it underlies macroscopic phenomena such as wetting and hydrophobicity, as well as several industrially relevant processes, including the operation of fuel cells and the activity of aqueous catalysts. While the degree of hydrophobicity/-philicity of graphene is currently being debated, it is commonly assumed that water wets graphene less than graphite due to reduced van der Waals interactions between the interfacial water molecules and the carbon sheet in the former, which in turn results in unfavorable (more positive) solid/liquid surface free energies. Here, by employing extensive computer simulations and analysis of the molecular correlation functions, we show that the interfacial water thermodynamics is in fact dominated by surface entropy, which is more favorable on graphite, due to increased population of low frequency librational modes. The signature of this effect is a red-shift in the interfacial water spectrum. The subtle interplay between librational entropy, binding and zero point energies in this system may have significant consequences for the design of graphene based, temperature sensitive, aqueous nanoscale devices.



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