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Spectral Investigation of Thermal Conductance at Solid/Fluid Interfaces

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Abstract:

As transistor power densities exceed 1 kW/cm², interfacial thermal conductance (G) at solid/liquid (SL) boundaries becomes a key bottleneck in two-phase cooling, comparable to bulk boiling or convection resistances. G is governed by nanoscale energy exchange, but the vibrational mechanisms involved, especially in SL interfaces, remain poorly understood. Common spectral metrics like the vibrational density of states (VDOS) often fail to predict G.

Using molecular dynamics simulations and spectral analysis, we examine three systems: (a) a basic Lennard-Jones interface, (b) the same interface with a nanochannel-confined meniscus, and (c) metal/water interfaces with tunable wettability. Across all cases, VDOS fails to capture G trends, while our new spectral metrics reveal key mechanisms, such as interfacial solidification, enhanced vibrational coupling from menisci, and material-specific spectral utilisation. These insights point to strategies for improving interfacial heat transfer, such as hydrophilic coatings or nanoscale confinement, with applications in high-power electronics, plasmonics, and other heat-intensive technologies.



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Biography:

Dr. Rohit Pillai is a Senior Lecturer (equivalent to Associate Professor) in Mechanical Engineering at the University of Edinburgh, where he co-leads the Multiscale Flow X Group (multiscaleflowx.github.io). His research focuses on computational thermofluid sciences, with an emphasis on nanoscale heat transfer and phase change.

He earned his PhD from the University of Melbourne in 2017 and joined University of Edinburgh in 2018. He has published in 20 articles (including in Physical Review Letters and Nano Letters), and has had his work featured by the BBC, The Times, Metro, and a radio interview on BBC Newsnight Scotland.

He has supervised five PhD students and two postdoctoral researchers, both now in permanent academic positions. His current work is funded a €1.5M ERC Starting Grant (NANO-COOL, 2024–2029) on nanomaterial-enhanced cooling technologies.

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