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**The Role of Partial Enthalpy in Thermal Conductivity Calculations for Nanofluids** MATTHEW EDWARDS, Princeton University, JOHN SHELTON, Carnegie Mellon University — Over the past decade, reports of significantly enhanced thermal conductivity in solutions of nanoscale particles (nanofluids) have elicited a great deal of interest due to the large number of applications for efficient heat transfer fluids. A common method for calculating the thermal conductivity of a nanofluid uses the autocorrelation of the microscopic heat flux (Green-Kubo formalism), which contains a correction for the net transport of enthalpy due to species diffusion. The partial enthalpy component of the correction term cannot be found from microscopic quantities and is often approximated by the partitioned enthalpy. Using NPT molecular dynamics simulations over a wide range of interaction energies, we show that this approximation leads to spurious enhancements with magnitudes similar to those reported in the literature. The discrepancy arises because the partitioned enthalpy neglects the change in fluid-fluid interaction enthalpy which occurs around solid particles; in systems with strong fluid-solid interactions this can be a substantial portion of the total enthalpy. This work suggests that the standard method for calculating thermal conductivity in nanofluids may be invalid and that actual conductivity enhancements are comparable to those predicted by Maxwell's theory.

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