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Heat Transfer in Porous Crystals Containing Adsorbed Gases
HASAN BABAEI, CHRISTOPHER WILMER, University of Pittsburgh — Using molecular modeling, we investigated heat transfer phenomena in a porous crystal containing gases. This study was motivated by the challenge of quickly dissipating heat generated in metal-organic frameworks (MOFs) during gas adsorption. Our study reveals that thermal conductance is dominated by lattice thermal conductivity in the crystal, and that conductance decreases as the density of gas in the pores increases. We show that the observed decreased conductivity is due to phonon scattering in the crystal due to interactions with gas molecules. We have also investigated the effect of pore size and shape on thermal transport in these structures. We show that thermal conductivity of pure nanoporous crystals decreases with pore size. For nanoporous crystals with small pores, gas adsorption reduces thermal conductivity due to more phonon scatterings, whereas for larger pores, the increase in gas loading does not affect lattice thermal conductivity. We show that the probability of gas-crystal collisions is smaller for larger pores, which explains why loaded gases do not significantly affect thermal conductivity of large pore structures.

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