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Thermal Transport Properties of Common Transition Single Metal Atom Catalysts

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Abstract : It is of great interest to investigate the thermal properties of non-precious metal catalysts for Proton exchange membrane fuel cell (PEMFC) based on the thermal management requirements. Due to the low symmetry of materials, to accurately obtain the thermal conductivity of materials, it is necessary to obtain the second and third order force constants by combining density functional theory and machine learning interatomic potential. To be specific, the interatomic force constants are obtained by moment tensor potential (MTP), which is trained by the computational trajectory of Ab initio molecular dynamics (AIMD) at 50, 300, 600, and 900 K for 1 ps each, with a time step of 1 fs in the AIMD computation. And then the thermal conductivity can be obtained by solving the Boltzmann transport equation. In this paper, the thermal transport properties of single metal atom catalysts are studied for the first time to our best knowledge by machine-learning interatomic potential (MLIP). Results show that the single metal atom catalysts exhibit anisotropic thermal conductivities and partially exhibit good thermal conductivity. The average lattice thermal conductivities of G-FeN_4, G-CoN_4 and G-NiN_4 at 300 K are 88.61 W/mK, 205.32 W/mK and 210.57 W/mK, respectively. While other single metal atom catalysts show low thermal conductivity due to their low phonon lifetime. The results also show that low-frequency phonons (0-10 THz) dominate thermal transport properties. The results provide theoretical insights into the application of single metal atom catalysts in thermal management.

Keywords : proton exchange membrane fuel cell, single metal atom catalysts, density functional theory, thermal conductivity, machine-learning interatomic potential
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