

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 and then further solve 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-FeN₄, G-CoN₄ and G-NiN₄ 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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