Recent Advances in Ab Initio Calculations of the Thermophysical Properties of Metals Near the Liquid-Gas Coexistence Curve

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We present our latest advancements in describing the thermodynamic, transport, and optical properties of metals from the vicinity of melting up to the critical point using the quantum molecular dynamics method. Our analysis focuses on some key metals of nuclear energy such as nickel, zirconium, and hafnium, examining their thermal expansion, enthalpy, resistivity, and normal spectral emissivity. We will demonstrate the calculated dependencies of density, enthalpy, isobaric and isochoric heat capacities, the Grüneisen parameter, and the speed of sound on temperature along the critical isobar for these metals. Additionally, we provide estimates of their critical parameters based on quantum molecular dynamics calculations of supercritical isotherms. The results of first-principles resistivity calculations for Zr, Hf, and Ni over a wide temperature range will also be discussed.
Furthermore, *ab initio* calculations of normal spectral emissivity for these metals in the liquid phase along the critical isobar will be presented.
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