First-principles calculation of resistivity and normal spectral emissivity for hafnium

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Hafnium is a chemically inert, refractory metal widely used in the nuclear industry. The resistivity and optical properties of hafnium at temperatures up to 10 kK have been studied using first-principles methods through quantum molecular dynamics simulations.
The Kubo–Greenwood formula was applied to determine the dynamic electrical conductivity. Based on the computed conductivity, the optical properties–such as normal spectral emissivity, reflectivity, and refractive index–were derived using the Kramers–Kronig transformation.
The influence of various exchange-correlation functionals on the calculated properties of Hf was analyzed.
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