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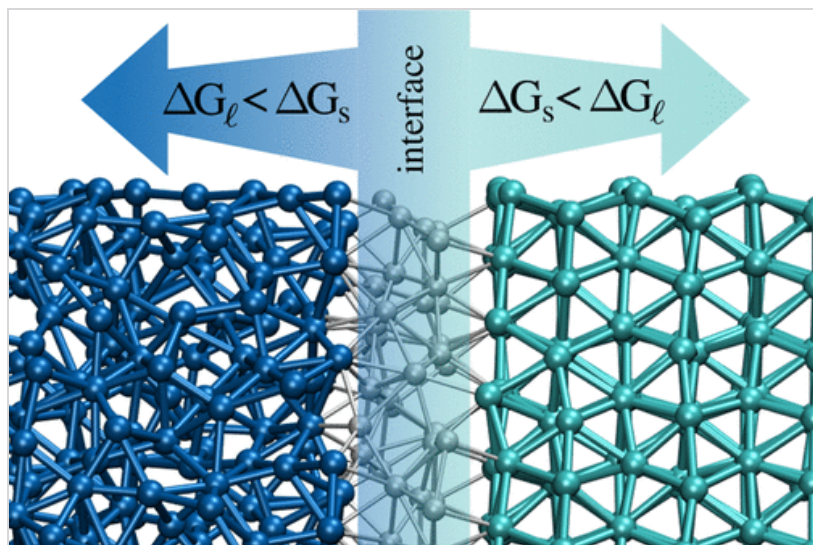
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LETTER | March 12, 2017

Accurate, Large-Scale Density Functional Melting of Hg: Relativistic Effects Decrease Melting Temperature by 160 K

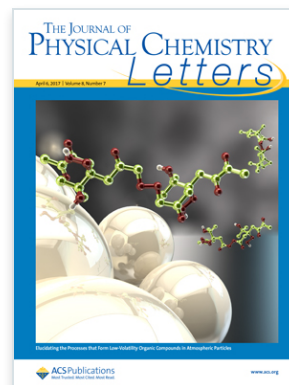
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Abstract



Using first-principles calculations and the “interface pinning” method in large-scale density functional molecular dynamics simulations of bulk melting, we prove that mercury is a liquid at room temperature due to relativistic effects. The relativistic model gives a melting temperature of 241 K, in excellent agreement with the experimental temperature of 234 K. The nonrelativistic melting temperature is remarkably high at 402 K.

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