From Metal to Insulator and Back Again: Transitions in Simple Metals

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Scientific Achievement

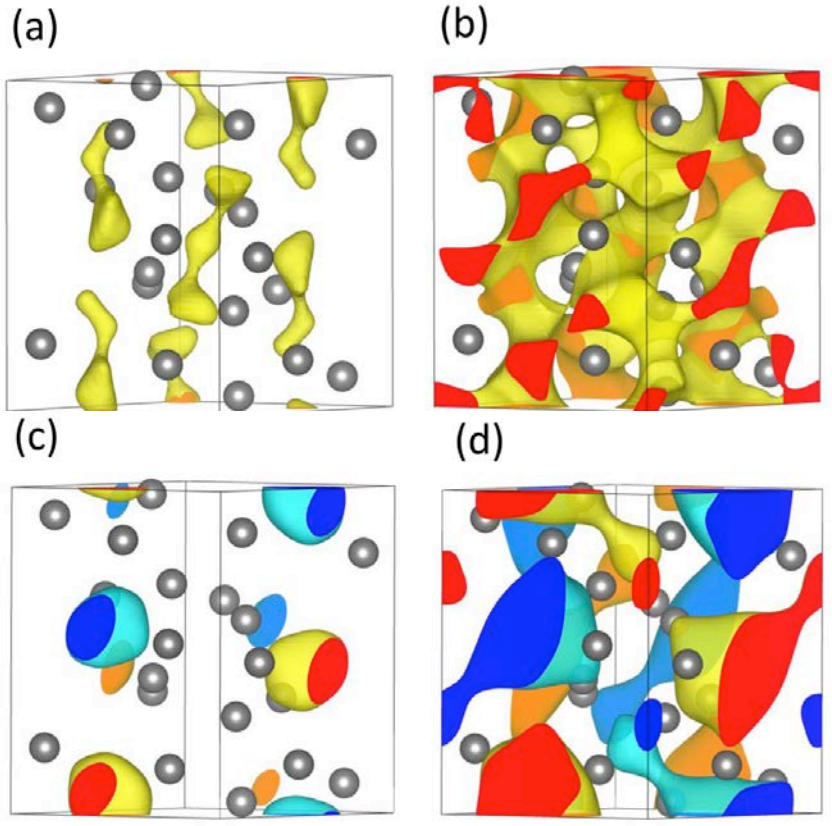
Development of unifying, symmetry-based principles that govern transitions between metallic and insulating states in simple metals

Significance and Impact

At high pressure, chemical bonding at *interstitial* sites in some solids creates insulating states. Understanding novel metal-insulator-metal transitions is crucial for predicting and confirming exotic behavior (e.g., superconductivity) at extreme conditions

Research Details

- First-principles calculations of band structures and charge densities of dense phases of Li, Na and Ca
- Combined pseudopotential and projector-augmented wave approach allows separation of valence *s*-states from atomic core states
- Group-theoretical analysis of band structure topology provides predictive rules about the occurrence of this unusual high pressure behavior



Representation of the valence band wave functions in Aba2-Li at 80 GPa. Spheres are nuclei, colors are electronic wave functions. (a, b) Bottom wave function. (c,d) Top wave function.

Naumov I. I. and Hemley R. J. Origin of Transitions Between Metallic and Insulating States in Simple Metals, Phys. Rev. Lett. **114**, 156403 (2015).

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