New Insights into Bonding in Low-Z Energy Materials: Hydrogen and Lithium Under Pressure

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Scientific Achievement

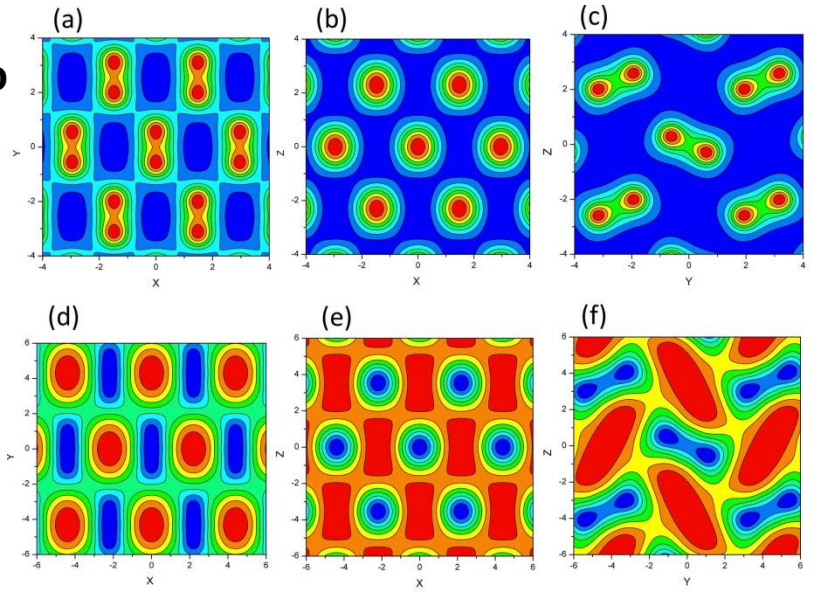
Detailed theoretical study reveals deeper understanding of differences and parallels in chemical behavior and physical of the two lightest neighbors in Periodic Table

Significance and Impact

Low-Z materials are now known to exhibit a broad range of new phenomena, including many that are ultimately important for energy applications. Despite a century of study, we show that aspects of the bonding in the 'simplest' solids, hydrogen and lithium, remain to be discovered. The results have implications for the search for new structures with novel properties such as high-T_c superconductivity.

Research Details

- First-principles calculations of band structures and charge densities of dense phases of H and Li
- The approach allows separation of valence *s*-states from atomic core states in Li
- Virial theorem is used to analyze the jumps in kinetic energy at the points of first-order pressure-induced phase transitions



Valence charge density in different cross sections for H (a,b,c) and Li (c,d,e) in the Cmca-4 structure. Hydrogen corresponds to Ω =8.68 Bohr^3 and 400 GPa, whereas Li to Ω =33.51 Bohr^3 and 130 GPa. (a,d) xy plane, (b,e) xz plane, and (c,f) xz plane.

Ivan I. Naumov, Russell J. Hemley, Roald Hoffmann, and N. W. Ashcroft . Chemical Bonding in Hydrogen and Lithium under Pressure, J. Chem. Phys. **143**, 064702 (2015).

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