Quasimolecules in Compressed Lithium

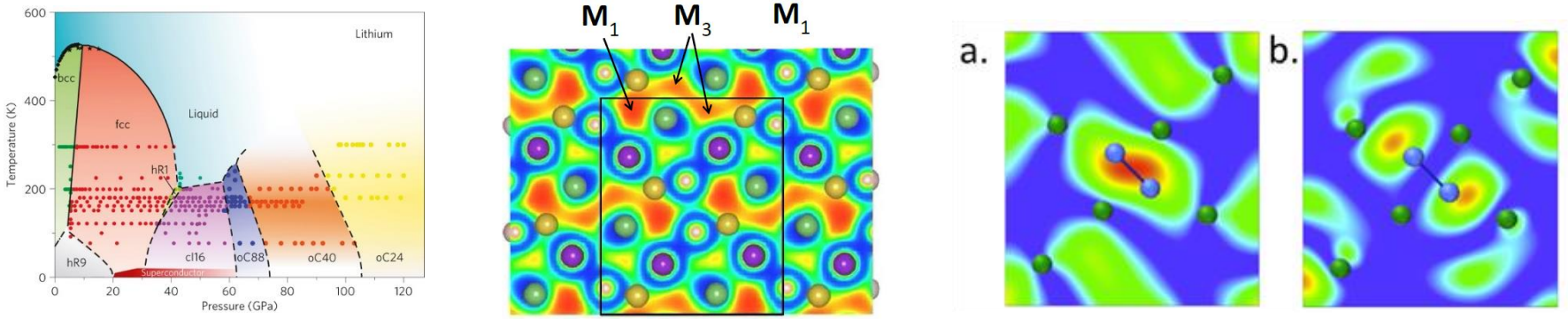
01/2017

Scientific Achievement

Theory indicates that under pressure electrons in insulating 'electride' phases of a "simple" metal, Li, can exhibit properties of isolated molecules within the structure.

Significance and Impact

A new kind of bonding is revealed in compressed materials, another way to understand their potential semiconducting behavior.



(left) Phase diagram of Li under pressure; (middle) one cross-section of electron density in Li Aba2 oC40 phase at 60 Gpa; here M_3 are the quasimolecule electron density positions; (right) focusing in on the quasimolecule; its σ and σ orbitals.*

Research Details

Miao, M. S., R. Hoffmann, J. Botana, I. I. Naumov, and R. J. Hemley, Quasimolecules in compressed lithium, *Agnew. Chem. Int. Ed.* **55**, 1 (2016).

- Structural relaxations and the electronic band-structure calculations were performed within the framework of density functional theory as implemented by the VASP code.
- Bonding was analyzed with crystal orbital Hamiltonian populations, electron density plots, and Wannier functions