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Quasimolecules in compressed Lithum[1] MAOSHENG MIAO, California State University, ROALD HOFFMANN, Cornell University, JORGE BOTANA, Beijing Computational Science Research Center, IVAN NAUMOV, Carnegie Institution of Washington, ROSSELL HEMLEY, The George Washington University —
Electrides are materials in which some valence electrons are separated from all atoms and occupy interstitial regions, effectively forming anions with no centering nuclei nor core electrons. Recently, it is found that, under high pressure, alkali metals such as Li and Na become semiconducting or insulating. As they do so, they adopt structures containing sites that accommodate electrons, leading to the formation of high-pressure electrides (HPE). Similar phenomena have also been predicted for Mg, Al and several other materials. The driving force for HPE formation may be attributed to the lack of core electrons in the interstitial sites, which causes the energies of the corresponding quantized orbitals to increase less significantly with pressure than normal atomic orbitals. These empty sites enclosed by surrounding atoms have been termed interstitial quasiatoms (ISQ); they may show some of the chemical features of atoms, including the potential of forming covalent bonds. Here we argue that some calculated ISQs in the high-pressure semiconducting Li phase (oC40, $Aba2$) actually form covalently bonded pairs. We suggest such quasimolecules may be found in other systems at high pressures as well.

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