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Compression effects on electrons for chemical bonding ANGUANG HU, FAN ZHANG, Defense R&D Canada-Suffield — How electrons move under compression as chemical bonds between atoms are broken and formed is central to a number of challenges on the performance of materials in extreme conditions. This is not only associated with the fundamental knowledge of material response to compressive loading but also would advance many aspects of material science towards future energy technologies. First-principles simulations of enthalpy minimization, in various target pressures on chemical transformation bonding pathways, reveal that high pressure can push electrons away from their denser regimes where the kinetic energy rises steeply on compression, causing a destabilization of intramolecular bonds. The high-pressure pushing of electrons from one regime to another thus leads to chemical bond destruction and formation with a cell volume collapse accompanied by a drop in stress components. Determination of such electron pathways following bonding conformations of molecular precursors would then result in a number of chemical transformations for novel materials, including high energy density materials.

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