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First-principles simulations on bonding pathways of chemical transformations under hydrostatic compression ANGUANG HU, FAN ZHANG, DRDC Suffield — High pressure as a thermodynamic parameter provides a strong structural constraint to lead chemical transformations with selective ways. Thus, chemical transformations under pressure can create novel materials which may not be accessible by covalent synthesis. However, bonding evolution toward high pressure chemical transformations can be a complex process and may happen over widely different pressures. To understand bonding evolution pathways of high pressure chemical transformations, first-principles simulations were performed following hydrostatic compression enthalpy minimization paths to obtain experimentally and theoretically established phase transitions of carbon. The results showed that the chemical transformations from hydrostatic compression carbon to single-bonded phases were characterized by a sudden decrease in principal stress components, indicating the onset of chemical transformation. On this basis, a number of hydrostatic compression chemical transformations from molecular precursors to novel materials were predicted, such as hydrocarbon graphane, a hydrogenated carbon nitride sheet, and carbon nitrides. All predicted hydrostatic compression transformations are featured as a sudden change in principal stress components, representing chemical bonding destruction and formation reactions with a cell volume collapse.

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