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**Bonding evolution towards phase transitions for nitrogen-rich high energy density solids under high pressure** ANGUANG HU, FAN ZHANG, Defence Research and Development Canada - Suffield — The evolution of chemical bonds towards phase transitions under high pressure can be a complex process and may happen over widely different pressures, depending on both bond strengths and structures. This often results in the formation of unexpected intermediate states and leads to difficulties on accurate predictions of phase transitions and experimental syntheses. To understand bonding evolution towards phase transitions under high pressure, first-principles simulations have been conducted for experimentally established phase transitions. The results reveal that the bonding evolution from a parent phase under high pressure is characterized by electron delocalization towards the direction of neighboring molecules. This process manifests itself by decreasing inter-molecular bond lengths while simultaneously stretching intra-molecular bond lengths. The dynamics of the electron delocalization leads to a volume collapse and the formation of a new phase which basically satisfies Lewis structures. On this basis, new nitrogen-rich high energy density solids, $C_3N_{12}$, $C_6N_{16}$, $N_4H_4$ and $N_2H_2$, are predicted together with their equations of state, pressure-enthalpy phase diagrams and metastability, as well as their molecular crystal precursors and high-pressure phase transition paths for experimental syntheses.

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