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Abstract for an Invited Paper
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Novel Molecular Alloys under Extreme Conditions¹

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Novel van der Waals binary compounds, composed by two different molecular solids such as Xe and H₂, H₂ and O₂, NH₃ and H₂, and CH₄ and H₂, are understood as “molecular alloys” in terms of a changing of coordination numbers or a formation of clathrate system which are comparable to the substitution or the occupation of atoms in the interstices of the host crystal lattice in metal alloy. Such molecular alloys show markedly differences in physical and chemical properties such as phase transitions, structural and electrical transition, optical changes, stiffness changes, and so on. In this presentation, three molecular alloys will be demonstrated. First, extended solid XeF₂ which transforms to novel two- and three-dimensional extended non-molecular phases and their metalization arising from a pressure-induced delocalization of non-bonded lone-pair electrons of F. Second, N₂-H₂ system which shows the presence of a novel incommensurate-like (N₂)₁₂D₂ system above 10 GPa and a non-crystalline δ -N₂-like non-crystalline solid that arises at the onset of solidification. Third, CO-D₂ system which shows small amount of D₂ stabilizes metastable polymeric CO at ambient conditions by forming O-D bonds which are playing a disproportionate effects on the non-bonded electron pairs of O.

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