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Pressure-induced transformations of confined diatomic molecules inside the one-dimensional channels BINGBING LIU, State Key Lab of Superhard Material, Jilin University — Studies of the control and manipulation of atoms/molecules and their assemblies generate remarkable new insights into how physical and chemical systems function. Confining iodine into single crystal zeolite AlPO4-5(AFI), which consists of, well packed, one-dimensional (1D) channels with homogeneous inner diameter of 0.73 nm, has been recently identified to be an effective way to create 1D (I2)n chains. Here, iodine and bromine doped AFI were obtained by a high temperature vapor method. The confined iodine and bromine inside the 1D channels are found to exist as molecular chains, as well as small amount of standing and lying neutral molecules. Using polarized Raman scattering measurement, synchrotron X-ray diffraction and theoretical calculations, we have discovered a unique transition dynamics of the confined species inside the 1D channel of AFI under pressure. The pronounced pressure-induced prolongation of molecular chains, pressure-induced rotation of the confined neutral molecules, and the abrupt transition in the vibrational frequency of the confined iodine due to the change of the interaction between the confined species and host wall have been observed.

Bingbing Liu
State Key Lab of Superhard Material, Jilin University

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