Poster

NEW SOLIDS BASED ON $B_{12}N_{12}$ FULLERENES

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In recent years BN fullerenes have been synthesized experimentally. As their carbon counterparts, these BN fullerenes could be assembled in molecular solids, but this possibility has been shortly studied in the literature. In this work we focus on the smallest synthesized BN fullerene, B12N12, which is built by squares and hexagons.
First, the interaction between two of these fullerenes has been analyzed, using the hybrids B3LYP and MPW1PW91 density functional methods. Two different interactions have been studied in the dimer, a square facing a square (s-s), and a hexagon facing a hexagon (h-h). In both cases a B is facing a N. The most stable dimer was found to be (s-s) facing, with covalent interactions between the monomers, but other dimers with weak interactions have been found as well, which opens possibilities of new systems, as in the case of fullerene dimers and solids. The solids resulting from the infinite repetition fo the characterized dimers were optimized, finding two different solids, with covalent and weak interactions between monomers, respectively. The solid with covalent interactions is a nanoporous material that is more stable by around 12 eV. Due to the nanoporous character of this solid it could be used for heterogeneous catalysis, molecular transport, etc. The SIESTA code with the GGA-PBE density functional method has been used for the solid state calculations.