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Many-body decomposition of the interaction energy in lowest beryllium clusters Be_{3-8}.

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We present the decomposition of interaction energies in beryllium clusters, Be_m, m=3─8, into a series of all possible non-identical m-particle non-additivities up to m=8. We analyse the role of the electron correlation and compare non-additivities resulting from DFT and MP2 energies with reference aug-cc-pVTZ CCSD(T) and CASPT2 calculations. Dominating non-additivity term is the four--body contribution (1,2). Five- and six-body terms are still quite large in Be_5 and Be_6 clusters but the total interaction energy in Be_6 is not significantly affected thanks to their cancellation. Clearly, non-additivities in Be clusters must be considered in constructing the interatomic potentials for investigations of the beryllium solid state. Any model based on pair and even three particle interactions is useless. Pair interactions are far from being dominating in the decomposition of the interaction energy into m─body terms since they represent weak dispersion forces, while the bonding character in higher clusters is more covalent. Binding energies increase with the size of the cluster, being higher than 1 eV per atom in Be_6. In CCSD(T) calculations of Be clusters we checked highest CC excitation amplitudes as indicators of possible effects of quasidegeneracy.

We have also considered $B_xC_yN_z$ species as a coverage for plasma facing materials. Using the VASP package with the DFT-D3BJ method we performed pilot calculations on the thermal stability and the band gaps of h-$C_m(BN)_n$ systems. The calculations indicate that thanks to a variety of possible BCN based species some of them may fulfill requirements for using in the fusion reactor as an alternative to existing materials.

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