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Towards a new two-dimensional ZnO monolayer from cluster Assembly[1] ANJALI KSHIRSAGAR, PRASHANT GAIKWAD, Department of Physics, Savitribai Phule Pune University , Pune 411 007, INDIA , SUDIP CHAKRABORTY, Materials Theory Division, Angstrom Laboratory Department of Physics and Astronomy, Uppsala University, Uppsala, SWEDEN , PRADEEP PUJARI, Radiochemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, INDIA — Two-dimensional structures, particularly of II-VI semiconductors, are being studied due to their technological applications stemming from their unique electronic properties. ZnO has been studied both experimentally and theoretically in bulk as well as in various nanostructured forms due to its wide band gap and large exciton energy. Monolayer ZnO has been recently synthesized experimentally and has been studied theoretically in hexagonal form. We propose a new octagonal ZnO monolayer, formed computationally by assembling stable geometries of passivated $(ZnO)_2$ and $(ZnO)_4$ clusters. The stability of the monolayer has been established via the total energy, formation energy, phonon dispersion and thermal properties. Detailed electronic structure calculations and analysis on the basis of site projected local density of states, partial charge density and Bader charge analysis bring out the changes in hybridization in comparison to the known hexagonal monolayer. These are attributed to difference in the coordination and bonding among the Zn and O atoms. Possible applications for gas sensing and water splitting will be discussed.

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