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Atomic structures of magic ZnSe clusters from first principles calculation[1] SACHIN P. NANAVATI, C-DAC, Pune University campus, Pune 411007, SHAILAJA MAHAMUNI, S.V. GHAISAS, University of Pune, Pune 411007, India, VIJAY KUMAR, Dr. Vijay Kumar Foundation, 1969, Sector 4, Gurgaon 122001, India — We report the atomic and electronic structures of *magic* $(ZnSe)_n$ (n = 13, 33, and 34) clusters, employing first principles technique based on a pseudopotential approach. These sizes are important as laser ablated plumes of ZnSe have clusters with (n) = 6, 13, 19, 23, & 33 ZnSe molecular units in high abundance suggesting their high stablity and magic behavior. Earlier we had predicted the atomic structures of these clusters to be filled cage structures with a Se centered 3-D structure for n = 13 and a cage/core structure for n = 33 & 34. In the later two cases, a core of Zn_5Se_5 and Zn_6Se_6, respectively, is enclosed by a $Zn_{28}Se_{28}$ cage to form a 3-D structure. In contrast to ZnSe clusters, ZnO clusters in this size range have empty cage structures. Therefore, we have performed further calculations using both, GGA-PBE and hybrid HSE06 type of exchange-correlation functionals that suggest that our conclusion for the size n = 13 remains unchanged, but for larger clusters of sizes n = 33 & 34, hollow cage stuctures made up of 4- and 6-membered rings of ZnSe, are energetically more favourable than the filled cage structures. We shall discuss the trends in the electronic structure, binding enery, and HOMO-LUMO gap, as we vary the ZnSe size.

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