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Atomic structures of 13-atom clusters by density functional theory HSIN-YI CHEN, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan — The 13-atom cluster structures of the alkaline metals, alkaline earth metals, boron group, 3d, 4d, and 5d transition metals in the periodic table, and Pb are investigated by density functional theory with three kinds of exchange correlation approximation: i) LDA (Local Density Approximation), ii) GGA (Generalized Gradient Approximation) [1], and iii) PBE (Perdew-Burke-Ernzerhof) [2]. The results mainly focus on five 3-D structures: icosahedral, cuboctahedral, hexagonal-closed packed, body-center cubic, decahedral, and the other two layer structures: buckled biplanar (bbp) and garrison-cap biplanar (gbp) structures. Limited by accuracy of exchange correlation approximation, two interesting results are found. The ground states of Ca_{13} , Sr_{13} , Ba_{13} , Sc_{13} , Y_{13} , La_{13} , Ti_{13} , Zr_{13} , and Hf_{13} are icosahedral structures. The clusters of Ir_{13} , Pt_{13} , Cu_{13} , Ag_{13} , and Au_{13} are more favorable for layer structures (i.e. bbp and gbp) than the other five 3-D structures.

[1] J. P. Perdew et al., Phys. Rev. B 46, 6671 (1992).

[2] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

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