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Structure and properties of chromium-sulphide (n=1-6) clusters

$Cr_n^{+/0/-}$ and $Cr_nS^{+/0/-}$

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In nanomaterials field the physical properties are strongly dependent on the size and the atomic environment. Many theoretical and experimental studies showed and quantified the strong dependence of magnetism with the local and chemical environment of the atoms and the dimensionnality of the system [1,2]. For its tendency to polarize antiferromagnetically, chromium remains a subject of study of topicality more especially as this clusters present properties far from being understood perfectly. This work concerns the study of the properties of chromium and chromium-sulphide clusters (n=1-6), in the neutral anion and cation states. Our calculations are carried out within the framework of the density functional theory implemented in VASP code. The effects of electronic exchange and correlation are treated in the generalized gradient approximation, with the functional of Perdew-Burke-Ernzerhof. We determine the geometrical structures of these small clusters and their magnetic and electronic properties (ionization potential, binding energy, electronic affinity,…). We will study the variation of the physical properties of pure chromium clusters according to their sizes as well as the effect of the insertion of a sulphur atom. The dimer-based growth pattern found in all considered low-lying isomers of neutral and anionic Cr clusters still persists in doped CrnS clusters. We found also that the elongation of Cr-Cr bonds upon the addition of the electronegative S dopant is not enough important to induce substantial influence on exchange coupling between the chromium atoms. In this communication, we will study the first four isomers. The results obtained are discussed in comparison with those of the experiments available.

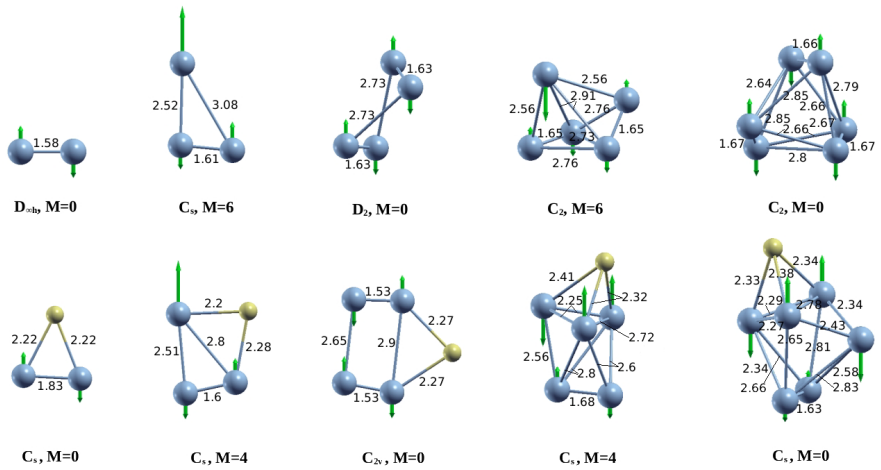

Figure : ground-state structures of neutral Crn and CrnS clusters with their symmetry and magnetic moment

References

[1] P. Ruiz-Diaz, J. L. Ricardo-Chavez, J. Dorantes-Davila, G. M. Pastor, PRB 81, 224431 (2010).

[2] Q. Wang, Q. Sun, B. K. Rao, P. Jena, Journal of Chemical Physics Vol 119 (14), 8 october (2003).