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**Clusters, Platelets, and Nanowires of Mo-S, and Their Assemblies**

P. MURUGAN, Central Electrochemical Research Institute, Karaikudi, T.N. India, VIJAY KUMAR, DR. Vijay Kumar Foundation, Gurgaon, India, Y. KAWAZOE, IMR, Tohoku Univ., Sendai, Japan, N. OTA, Hitachi Maxell Ltd., Tokyo, Japan — Nano-structures of MO-S are useful for removal of S in petroleum industry, as solid state lubricants in space technology, and in Pt-free fuel cell research. We study by first principles density functional calculations Mo-S nanoclusters, nanowires, their assemblies, and triangular nano-platelets all of which have been produced in laboratory. Mo-S clusters have Mo polyhedral structures and sulfur atoms cap this metal polyhedron. These structures have high stability due to strong Mo-Mo and Mo-S bonding. Some of the polyhedral clusters have non-zero magnetic moments due to the partially occupied 4d states in Mo atoms.  $\text{Mo}_6\text{S}_8$  octahedral cluster has ultra-high stability and it could be condensed to form Mo-S nanowire or nanorod. However, for high S contents, we show that triangular platelets become more stable. The Mo-S nanowires are good electronic conductors and are interesting for miniature devices. Assembly of nanowires stabilizes in a hexagonal structure with vdW interactions. The trigonal void between the nanowires can be occupied by Li atoms to develop materials for Li-ion battery applications. References: P. Murugan, V. Kumar, Y. Kawazoe, and N. Ota, Appl. Phys. Lett. (2008); Nano letters. (2007); J. Phys. Chem. A (2007).

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