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Induced super-halogen behavior of metal moieties in halogen-doped metal clusters FEDOR NAUMKIN, Faculty of Science, UOIT, Oshawa ON L1H 7K4, Canada, HOBART LEUNG — Recent studies of the $Al_{13}I^-$ cluster ion have shown negative charge localization on the aluminum core and associated this with its super-halogen character resulting from a high electron affinity EA of Al_{13} (exceeding that of the I atom). The present work reports results of ab initio calculations for a similar halogen-doped metal cluster, $M_{13}X^-$. The charge is found to be localized on the M_{13} core as well, even though its EA is lower than that of X. Other properties such as structure and stability for different spin-states are also investigated and compared with those for the neutral counterparts. Comparison to the corresponding smaller metal-halide species is made as well. The charge localization on the metal moieties is concluded to be associated not only with the relative EA values. An alternative, physically transparent interpretation is given, which explains the observed charge distributions on electrostatic basis. The super-halogen behavior of the metal moieties is linked to the presence of the halogen atom in the systems.

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