ELECTRONIC TRANSITIONS IN ANION PHOTOELECTRON SPECTRA OF VC_2^- AND $ScSi_2^-$

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Several levels of theory including single reference and multireference quantum wave function types (DFT, RCCSD(T), CASSCF/CASPT2 and MRCI) are synergistically used to investigate the electronic structures of $VC_2^{-/0}$ and $ScSi_2^{-/0}$. On the basis of electronic structures, possible one-electron ionization processes, which are the removals of one electron from anionic clusters, are predicted. Ionization energies of these transitions, the so-called adiabatic and vertical detachment energy (ADE and VDE), are also calculated at several levels of theory mentioned above. These calculated ADEs and VDEs provide reliable evidences to understand nature of all experimental photoelectron bands in the spectra. In addition, multidimensional Franck-Condon simulations are employed to confirm electronic transitions and/or provide more details about experimental results.

Keyword: Clusters, transition metals, anion, photoelectron, excited state, ground state