Abstract Submitted
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Ab initio **calculations for the photoelectron spectra of transition metal clusters**[1] SHEN LI, MANUEL ALEMANY, JAMES CHELIKOWSKY, University of Minnesota — We present results for negatively charged transition metal clusters Cu_n^- and V_n^- using *real-space* pseudopotentials constructed within the local spin density approximation. Our method assumes no explicit basis; wave functions are evaluated on a uniform grid. Only one parameter, the grid spacing, is used to control convergence of the electronic and structural properties of the cluster. To compare with experimental photoelectron spectra, we calculated the density of states (DOS) and the electron binding energies for the lowest energy structures. We found that for larger clusters (more than 5 or 6 atoms), the DOS can give reasonable agreement with experiment. However, for smaller clusters, the DOS fails to reproduce experiment. In contrast, we found that the constrained density functional method of Massobrio, Pasquarello and Car (Phys. Rev. Lett. **75**, 2104 (1995)) works very well for these smaller clusters.

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