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Surface core level shifts of germanium in the presence of alkaline-earth metals ALI HAMZE, Univ of Texas at Austin, Dept of Physics, SHEN HU, EDWARD LIN, Univ of Texas at Austin, Dept of Chemical Engineering, AGHAM POSADAS, Univ of Texas at Austin, Dept of Physics, HSINWEI WU, Arizona State Univ, Tempe, School of Engineering for Matter, Transport and Energy, DAVID SMITH, Arizona State Univ, Tempe, Dept of Physics, JOHN EKERDT, Univ of Texas at Austin, Dept of Chemical Engineering, ALEX DEMKOV, Univ of Texas at Austin, Dept of Physics — The integration of perovskites on semiconductors for use as gate oxides in field-effect transistors has been of interest due to their high dielectric constants. Since it was found that .5 monolayer (ML) of strontium on silicon allows for the epitaxial growth of perovskites on silicon, many studies of the growth of perovskites have been carried out on silicon and other semiconductors, such as germanium and gallium arsenide. In this work, we investigate the surface core level shifts (SCLSs) of the germanium 3d core level in the presence of .5 ML of the alkaline-earth metals (AEMs) barium and strontium using density functional theory. Results found using the local density approximation and generalized gradient approximation to the exchange-correlation energy, different valence electron configurations, and for various slab surface areas are compared to each other and to x-ray photoemission spectroscopy (XPS) data. We find the germanium surface dimers flatten in the presence of .5 ML of AEMs, forming a Zintl layer, in agreement with experiment. We also find the surface core levels shift towards lower binding energy, and that the shift is the same for all the surface atoms, in qualitative agreement with the XPS data.

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