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A theoretical investigation of selected silicides and germanides MANISH NIRANJAN, LEN KLEINMAN, ALEXANDER A. DEMKOV, The University of Texas — A germanium channel field effect transistor (FET) is being considered for the next generation CMOS technology. New material system requires re-development of most elements of the device. Low resistance contacts compatible with a self aligned process have to be developed based on metal germanides, and germanides with low n- and p-type Schottky barriers (for the use in NMOS and PMOS devices) to germanium channel need to be identified. We report a comprehensive theoretical study within the framework of density functional theory of several germanides (NiGe, PtGe, YGe, Y_5Ge_3, HfGe and $HfGe_2$) and compare them with monosilicides of Pt and Ni. We report bulk electronic structure and elastic properties. However, we focus on the surface properties important to thin films such as surface energy, work function and Schottky barrier height. We are able to identify thermodynamic stability fields for surface terminations resulting in work functions consistent with the low Schottky barrier requirement. Several interface structure were also considered which afford a direct evaluation of the barrier height. Germanides have complex phase diagrams, and we find *ab-initio* calculations extremely useful in providing fundamental understanding of the structure-property relations between the crystal structure, chemical composition and atomic structure of the alloy/semiconductor interface on one hand and the Schottky barrier height on the other hand.

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