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A Green Function Approach to the Effects of Core-state Overlap on Interatomic Interactions at Extreme Densities YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — Under extreme conditions of temperature and pressure, interatomic separations in condensed matter can approach a small fraction of those under normal laboratory conditions. For example, during high-energy ($\sim$ 100 keV) radiation damage cascades, interatomic separations can be as small as 0.5Å. Under such conditions, core states between neighboring atoms could overlap and must be included as band states. Here we use Greens function method in the framework of multiple scattering theory, also known as Korringa-Kohn-Rostoker (KKR) electronic structure methods, to seamlessly integrate these core overlap effects within an all-electron ab initio approach. To accomplish these we use multiple integration contours in the complex plane that incorporate states normally treated as bound atomic levels. We show results for Ni and NiFe alloys in extreme densities ($a/a_0 \sim 0.3$) to illustrate the convergence of the method with respect to which core states are banded as well as the angular moment cut-off required to establish absolute convergence of the total energies. Results are compared with those of plane-wave methods for different choices of the underlying pseudo potential to establish the range of validity of the various approaches.

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