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Ion-Ion Interactions in Simple Metallic Systems: Beyond Linear Response[1] JAMES PORTER, Dept. of Physics and Astronomy, Colby College, NEIL ASHCROFT, GEOFFREY CHESTER, Laboratory of Atomic and Solid State Physics, Cornell University — We extend the formalism of electronic response theory to second order in perturbing pseudopotentials and examine the physical consequences on effective ionic pair potentials for certain simple metals, under standard conditions. The pseudopotentials, assumed to be transferable, are of the Ashcroft empty-core form. Our results show that inclusion of second-order response terms in the pair potentials leads to the deepest potential minima having locations that are within 8% of the experimental nearest-neighbor distances for crystalline sodium, magnesium, aluminum, and metallic silicon, all in their standard one-atmosphere structures. Second-order response effects are found to become increasingly important as the valence increases. We briefly discuss two natural extensions of this research, namely to three-body potentials and to changes expected in pair potentials at higher densities.

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