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Tests on novel pseudo-potentials generated from diffusion Monte Carlo data.[1] FERNANDO REBOREDO, Oak Ridge National Laboratory, RANDOLPH HOOD, Lawrence Livermore National Laboratory, MICHAL BAJDICH, Lawrence Berkeley National Laboratory — Since Dmitri Mendeleev developed a table in 1869 to illustrate recurring ("periodic") trends of the elements, it has been understood that most chemical and physical properties can be described by taking into account the outer most electrons of the atoms. These valence electrons are mainly responsible for the chemical bond. In many ab-initio approaches only valence electrons are taken into account and a pseudopotential is used to mimic the response of the core electrons. Typically an all-electron calculation is used to generate a pseudopotential that is used either within density functional theory or quantum chemistry approaches. In this talk we explain and demonstrate a new method to generate pseudopotentials directly from all-electron many-body diffusion Monte Carlo (DMC) calculations and discuss the results of of the transferability of these pseudopotentials. The advantages of incorporating the exchange and correlation directly from DMC into the pseudopotential are also discussed.

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