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Classical multielectron model atoms with optimized ionization energies XU WANG, JIE ZHOU, Graduate School of China Academy of Engineering Physics — Semiclassical simulations are widely used alternative approaches to many-particle systems which have been long-standing challenges for quantum mechanics. Widely known examples include molecular dynamics simulations for proteins and particle-in-cell simulations for plasmas. Strong-field atomic physics is another area where classical simulations play an important role. Many insights about the atomic ionization process, especially double or multiple ionization processes, are obtained with classical simulations. A classical multielectron model atom, however, suffers two problems. The first problem is that the atom is not stable. The second (less known and more subtle) problem is incorrect ionization energies. In this presentation, we propose a method to build stable classical multielectron model atoms with the ionization energies optimized to experimental values. Based on the work of Kirschbaum and Wilets [Phys. Rev. A 21, 834 (1980)], which introduces auxiliary potentials to simulate quantum mechanical effects, we implement a genetic algorithm to optimize the related parameters such that the model atoms yield correct (first few) ionization energies. Ionization-energy optimized model atoms automatically show separated electron shells, consistent to normal expectations. Numerical examples are given to demonstrate the importance of correct ionization energies, as well as new perspectives to double ionization processes.

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