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Density-Functional Theory with Optimized Effective Potential and Self-Interaction Correction for the Double Ionization of He and Be Atoms[1] JOHN HESLAR, National Taiwan University, Taiwan, DMITRY TELNOV, St. Petersburg State University, Russia, SHIH-I CHU, University of Kansas — We present a *self-interaction-free* (SIC) time-dependent density-functional theory (TDDFT) for the treatment of double ionization processes of many-electron systems. The method is based on the Krieger-Li-Iafrate (KLI) treatment of the *optimized effective potential* (OEP) theory and the incorporation of an explicit self-interaction correction (SIC) term. In the framework of the time-dependent density functional theory, we have performed 3D calculations of double ionization of He and Be atoms by strong near-infrared laser fields. We make use of the exchange-correlation potential with the integer discontinuity which improves the description of the double ionization process. We found that proper description of the double ionization requires the TDDFT exchange-correlation potential with the discontinuity with respect to the variation of the spin particle numbers (SPN) only. The results for the intensity-dependent probabilities of single and double ionization are presented and reproduce the famous "knee" structure.

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