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Fully numerical all-electron solutions of the optimized effective potential equation for diatomic molecules ADI MAKMAL, Weizmann Institute of Science, Israel, STEPHAN KUMMEL, University of Bayreuth, Germany, LEEOR KRONIK, Weizmann Institute of Science, Israel — We present an approach for fully numerical, all-electron solutions of the optimized effective potential equation within Kohn-Sham density functional theory for diatomic molecules. The approach is based on a real-space, prolate-spherical-coordinate grid for solving the all-electron Kohn-Sham equations and an iterative scheme for solving the optimized effective potential equation. The accuracy of this method is demonstrated by comparison with previously reported calculations and new benchmark fully numerical results for selected dimers are provided.

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