

Abstract Submitted
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Correlated Light-Matter Interactions in Cavity QED JOHANNES

FLICK, Fritz-Haber-Institut, Berlin, CAMILLA PELLEGRINI, Universidad del Pais Vasco, San Sebastian, MICHAEL RUGGENTHALER, Institut für Theoretische Physik, Universität Innsbruck, HEIKO APPEL, Fritz-Haber-Institut, Berlin, ILYA TOKATLY, Universidad del Pais Vasco, San Sebastian, ANGEL RUBIO¹, Universidad del Pais Vasco San Sebastian — In the last decade, time-dependent density functional theory (TDDFT) has been successfully applied to a large variety of problems, such as calculations of absorption spectra, excitation energies, or dynamics in strong laser fields. Recently, we have generalized TDDFT to also describe electron-photon systems (QED-TDDFT) [1,2]. Here, matter and light are treated on an equal quantized footing. In this work, we present the first numerical calculations in the framework of QED-TDDFT. We show exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical high-Q cavities and coupled to quantized electromagnetic modes. We focus on the electron-photon exchange-correlation (xc) contribution by calculating exact Kohn-Sham potentials using fixed-point inversions and present the performance of the first approximated xc-potential based on an optimized effective potential (OEP) approach.

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¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, and Fritz-Haber-Institut der MPG, Berlin

Johannes Flick
Fritz-Haber-Institut der MPG, Berlin

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