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Cavity-QED beyond model systems — ●CHRISTIAN SCHAEFER¹, JOHANNES FLICK¹, HEIKO APPEL¹, CAMILLA PELLEGRINI², and ANGEL RUBIO^{1,2} — ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ²Nano-bio Spectroscopy Group and ETSF, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastian, Spain

The optimized effective potential (OEP) is a natural connection between local density-functional theory and Many-body perturbation theory. In principle, this variationally best local potential reduces the problem to solving a system of one-particle Kohn-Sham equations combined with the solution of the OEP integral equation. The Krieger-Li-Iafrate (KLI) approximation reduces the integral equation to an analytically solvable one via a dominant orbital approximation.

In the present work, we extend the OEP [1] and KLI approaches to the case of electron-photon interactions in cavity quantum electrodynamics. Here an effective electronic interaction is transmitted via transversal photons. We present first results for KLI and OEP derived from an effectively reformulated Sternheimer response equation [2].

With these approaches, we are able to determine the influence of the quantized electromagnetic field on the electronic configuration of realistic molecules described fully real-space resolved [2,3].

References:

- [1] C. Pellegrini et al., Phys. Rev. Lett. **115**, 093001 (2015).
- [2] J. Flick et al., in preparation
- [3] C. Schaefer et al., in preparation

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