Supplemental Materials: Intermolecular interactions in optical cavities: an ab initio QED study

Tor S. Haugland,[1] Christian Schäfer,[2] Enrico Ronca,[3,2] Angel Rubio,[2,4,5] and Henrik Koch[6,1]

[1)] *Department of Chemistry, Norwegian University of Science and Technology, 7491 Trondheim, Norway*

[2)] *Max Planck Institute for the Structure and Dynamics of Matter and Center Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany*

[3)] *Istituto per i Processi Chimico Fisici del CNR (IPCF-CNR), Via G. Moruzzi, 1, 56124, Pisa, Italy*

[4)] *Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth avenue, New York NY 10010.*

[5)] *Nano-Bio Spectroscopy Group, Departamento de Física de Materiales, Universidad del País Vasco, 20018 San Sebastian, Spain*

[6)] *Scuola Normale Superiore, Piazza dei Cavalieri, 7, 56124 Pisa, Italy*

I. ADDITIONAL DATA FOR VAN DER WAALS BONDS

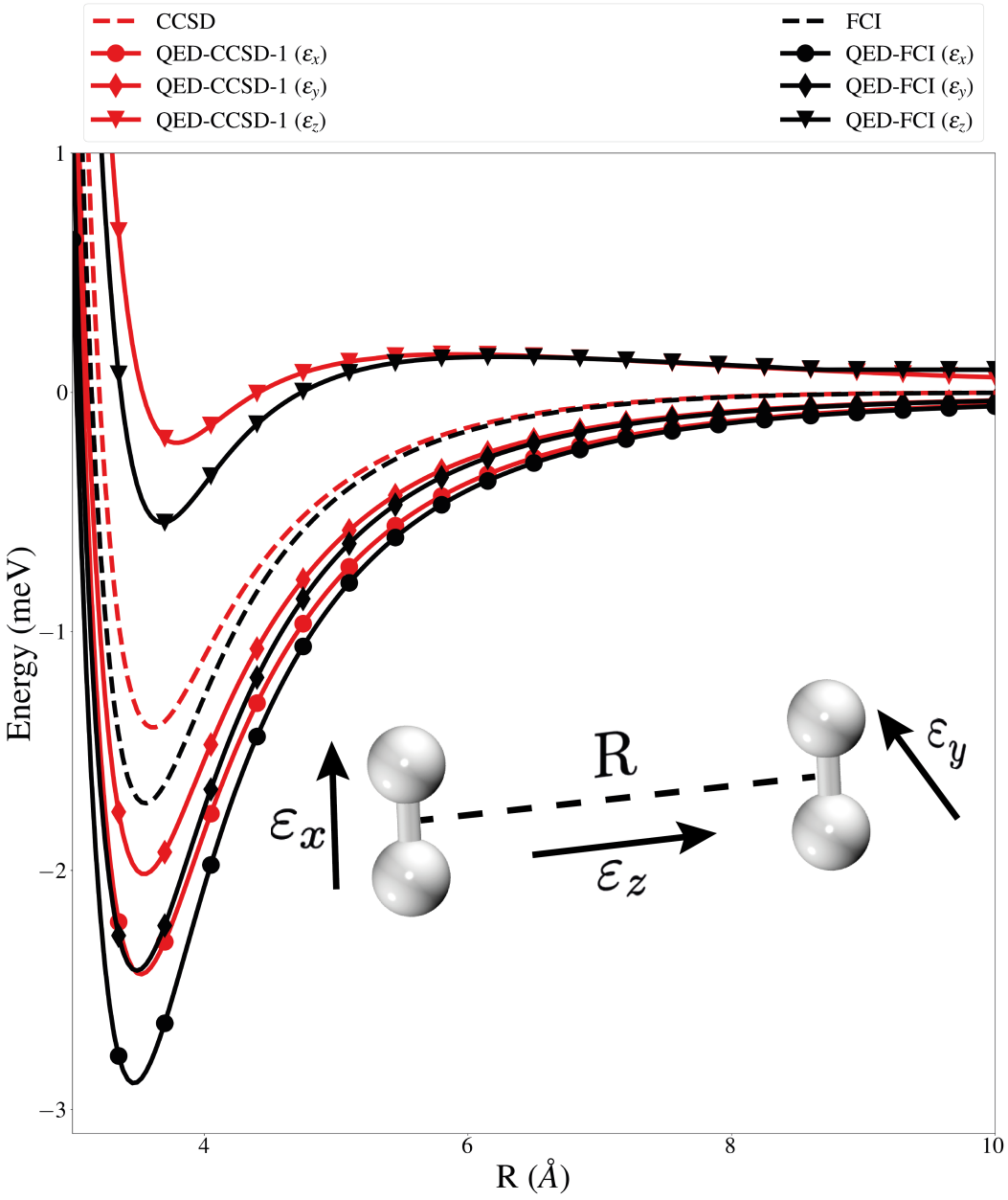

FIG. 1. $(H_2)_2$ polarization along H-H bond, orthogonal and along the chain.

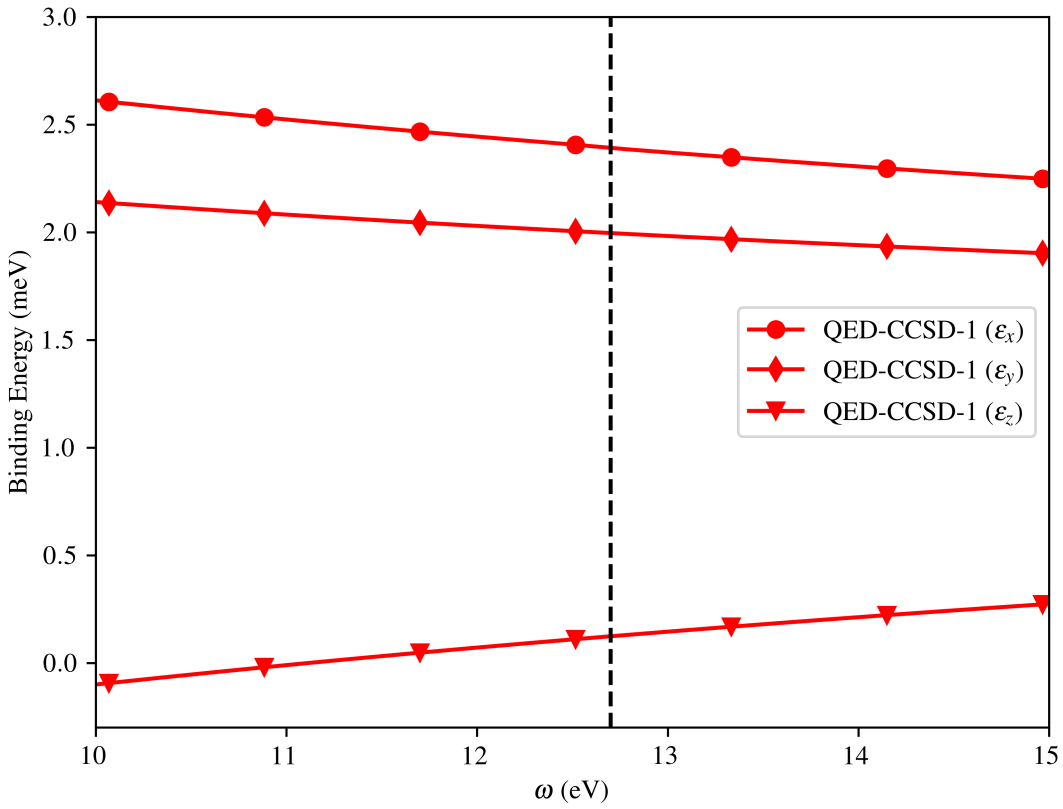

FIG. 2. Binding energy of two parallel H_2 molecules as a function of the photon frequency. Binding energies are calculated as energy differences between the value at 20 Å and 3 Å. The coupling value is set to $\lambda = 0.1$ and all three polarization directions have been presented. The black dashed line is the resonance frequency (12.7 eV).

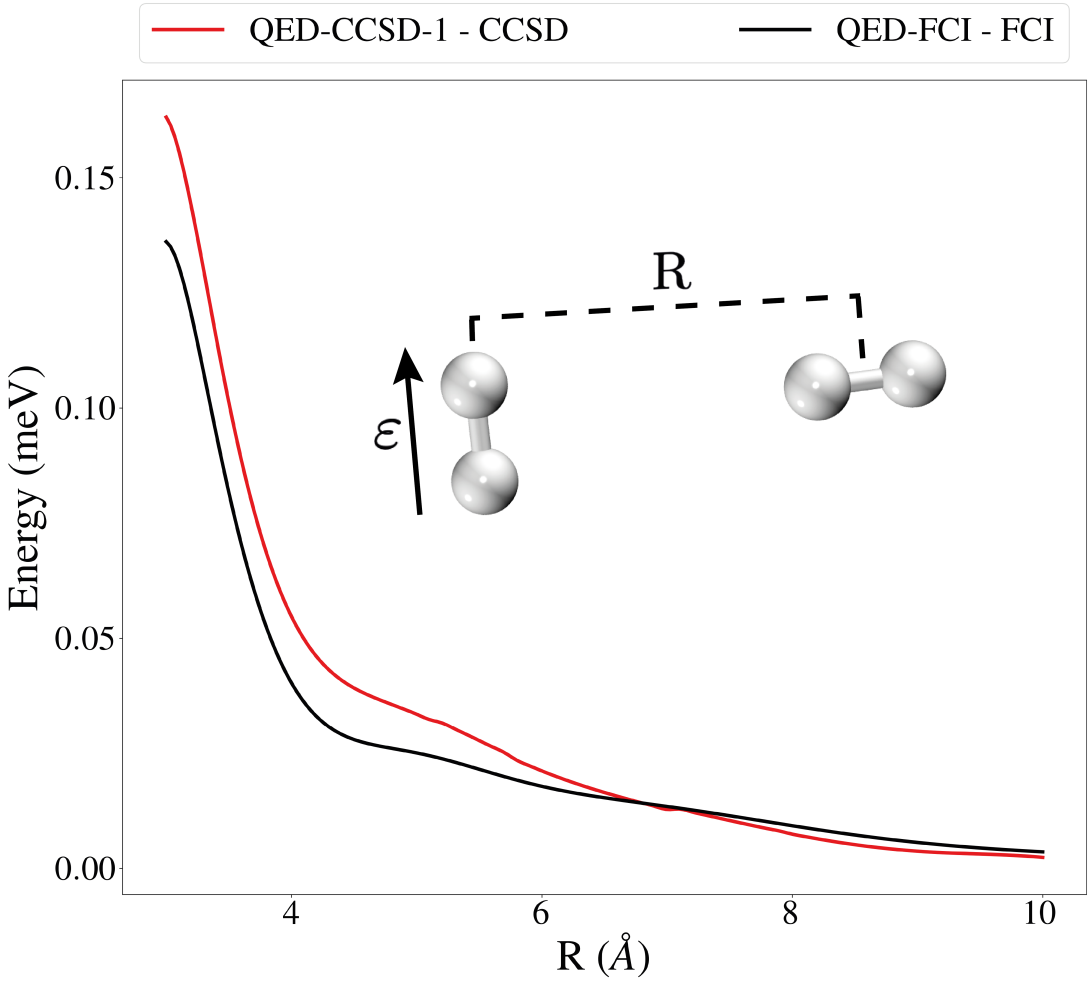

FIG. 3. Cavity induced effects on potential energy curves for two H_2 molecules in C_{2v} configuration stretching the distance between them. The polarization has equal components along the bond, chain and orthogonal directions with coupling $\lambda = 0.1$ and frequency $\omega = 12.7$ eV. The value at 200 Å has been subtracted.

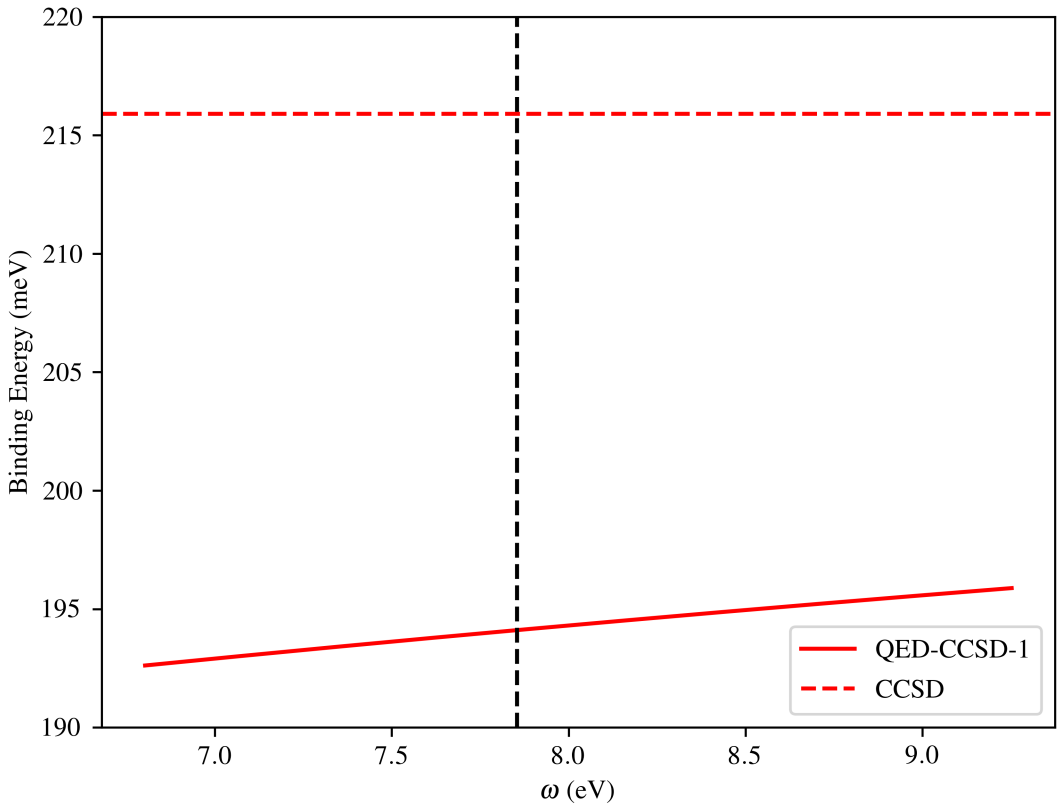

FIG. 4. Binding energy of the H_2O dimer as a function of the photon frequency. Binding energies are calculated as energy differences between the value at 20 Å and 3 Å distance between the oxygen atoms. The coupling value is set to $\lambda = 0.1$ and the polarization is parallel to the oxygens. The black dashed line is the resonance frequency (7.86 eV).