

## Electronic Supplementary Information

# Voronoi dipole moments for the simulation of bulk phase vibrational spectra

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## 1 Raman spectrum of phenol

In addition to the AIMD simulation discussed in the article, the Raman spectrum of phenol was also estimated by static calculations of a single molecule using three different exchange-correlation functionals. The software package ORCA 3.0.2 [1] was used to carry out the DFT calculations within the RI approximation [2, 3], applying a polarized triple-zeta basis set (def2-TZVPP) to all atoms [4, 5], and utilizing the BLYP [6, 7], TPSS [8], and B3LYP [9] exchange-correlation functionals with Grimme's dispersion correction D3 [10]. For all three functionals, a geometry optimization was performed, and vibrational frequencies were determined by numerical second derivatives. Polarizabilities for Raman intensities were calculated analytically. The obtained line spectra were broadened by Lorentzian functions with a full width at half maximum of  $15\text{ cm}^{-1}$ .

Apart from slight shifts of the vibrational frequencies, all three exchange-correlation functionals show very similar spectra (see figure S1). The region below  $3000\text{ cm}^{-1}$  is in good agreement with the bulk phase spectrum from the AIMD simulation, but the static calculations of a single molecule do not include the bulk effects on the O-H stretching mode, which is strongly influenced by intermolecular hydrogen bonds. Most importantly, all functionals, which were selected from a wide range of possibilities (GGA, meta-GGA, hybrid), show a similarly large intensity of the C-H stretching modes. This indicates that the overestimation of the Raman intensity above  $3000\text{ cm}^{-1}$  in the bulk simulation is not connected to the particular choice of the BLYP functional, but is a more general issue of DFT.

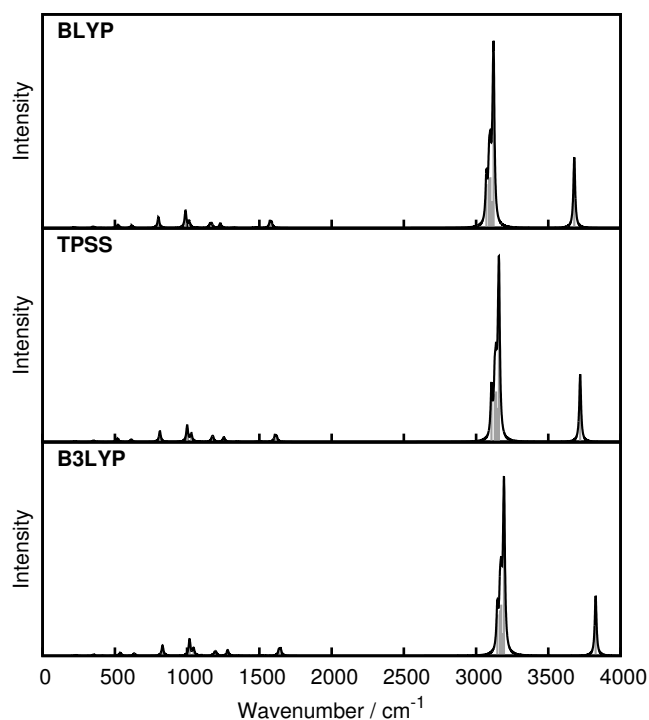


Figure S1: Raman spectrum of phenol by static calculations with three different exchange-correlation functionals. The lines were broadened by Lorentzian functions with a full width at half maximum of  $15 \text{ cm}^{-1}$ .

## 2 XYZ coordinates of initial structures

### 2.1 Methanol

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## 2.2 Benzene

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