First Principle Molecular Dynamics Investigation of Waterborne As−V Species

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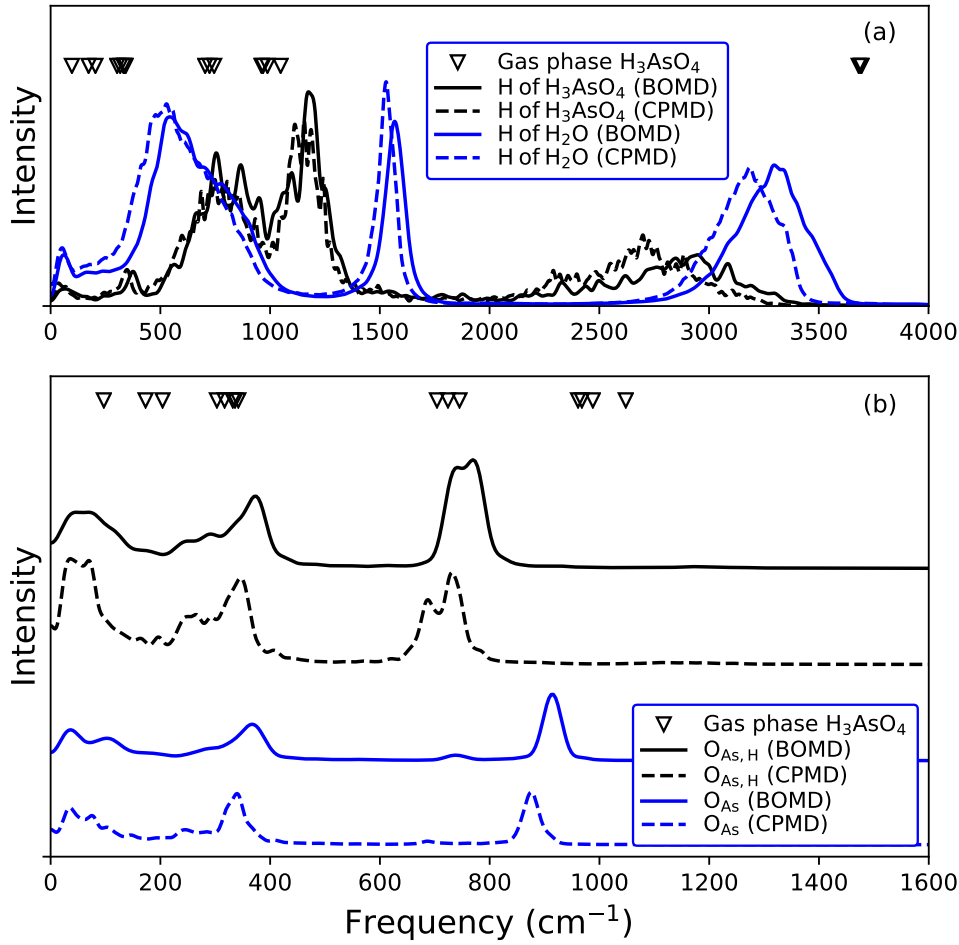
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Figure S1: The vibrational density of states (VDOS) from CPMD (dotted lines) simulation is compared with Born-Oppenheimer (BO) MD (solid lines). Top panel (a): H of H_3AsO_4 (black) and H of H_2O (blue); Bottom panel (b): $O_{As,H}$ (black) and O_{As} (blue) atoms of H_3AsO_4. The gas phase vibrational frequencies are shown in both panels as triangles pointed-down.

The shifts of CPMD spectra w.r.t. the BOMD ones are approx. 110 cm^{-1} for OH stretching modes of H_2O and approx. 240 cm^{-1} for those of H_3AsO_4 (intra-molecular), while for $As-O_{As}$ and $As-O_{As,H}$, those are approx. 40 cm^{-1}. The BOMD simulations are carried out at 315 K starting from a well equilibrated structure of one H_3AsO_4 solvated by 60 H_2O molecules in box of size 12.42 Å. These calculations are performed at the same level of theory as the CPMD simulations, except that a larger time steps of 0.25 fs is used, and the total run is 6 ps long.