

# Supplementary Information: Title

Joseph Heindel<sup>1,2</sup>, Teresa Head-Gordon<sup>1,2,3</sup>

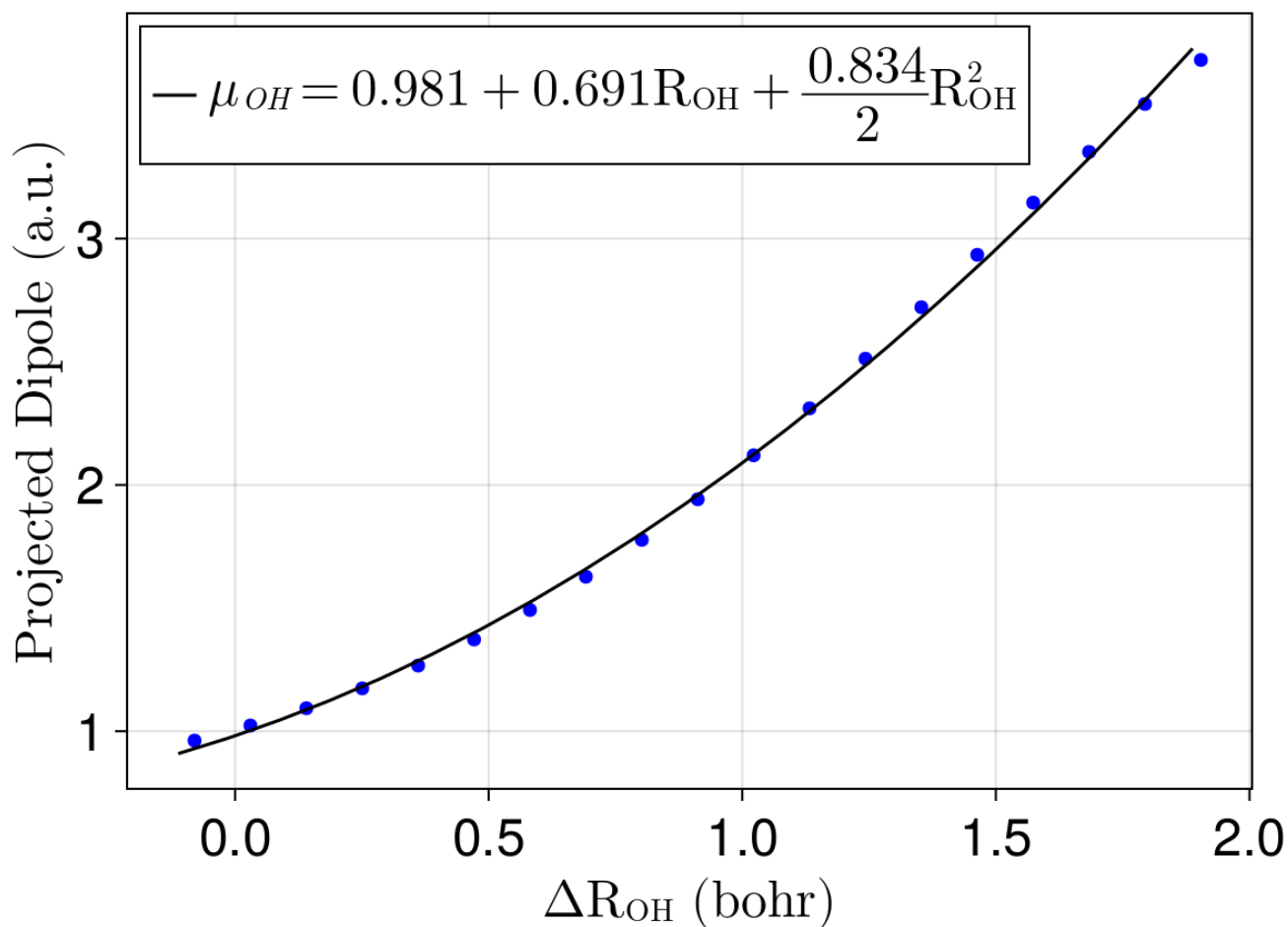
<sup>1</sup>Kenneth S. Pitzer Theory Center and Department of Chemistry

<sup>2</sup>Chemical Sciences Division, Lawrence Berkeley National Laboratory

<sup>3</sup>Departments of Bioengineering and Chemical and Biomolecular Engineering

University of California, Berkeley, CA, USA

corresponding author: thg@berkeley.edu



**Supplementary Figure 1:** *Projected dipole moment of water dimer O-H stretch* The dipole moment of  $(H_2O)_2$  is computed with  $\omega B97X-V/def2-QZVPPD$  as a function of the O–H stretch distance. All other degrees of freedom are fixed. The dipole moment is projected along the O–H stretch unit vector. The second order polynomial fit allows us to read off the corresponding dipole derivatives needed in the evaluation of the field-dependent morse potential.

## 9 Supplementary References