

The scatter and contour plots below show 2-body interaction energies

$$E_{2B}(x_1, x_2) = E(x_1, x_2) - E(x_1) - E(x_2),$$

for the water dimers computed using model potentials (CCpol-8sf, HBB2 and MB-pol) in comparison to the CCSD(T)/CBS values for each of the four components of the MB-pol short-range training set. Contour plots visualize the density of the points shown in the corresponding scatter plots. The density was computed as follows:

$$\rho(E_{ref}, E_{model}) \propto \sum_{a \in S} \exp \left[ -\frac{(E_{ref}^{(a)} - E_{ref})^2 + (E_{model}^{(a)} - E_{model})^2}{2\sigma^2} \right],$$

where the sum runs over all dimers whose energies fall inside the region shown in a particular plot. Here,  $E_{ref}^{(a)}$  and  $E_{model}^{(a)}$  denote the reference and model energy values for the  $a$ -th dimer,  $\sigma$  was set to 0.1 kcal/mol and  $\rho$  was normalized to integrate to unity over the area shown in the corresponding plot.

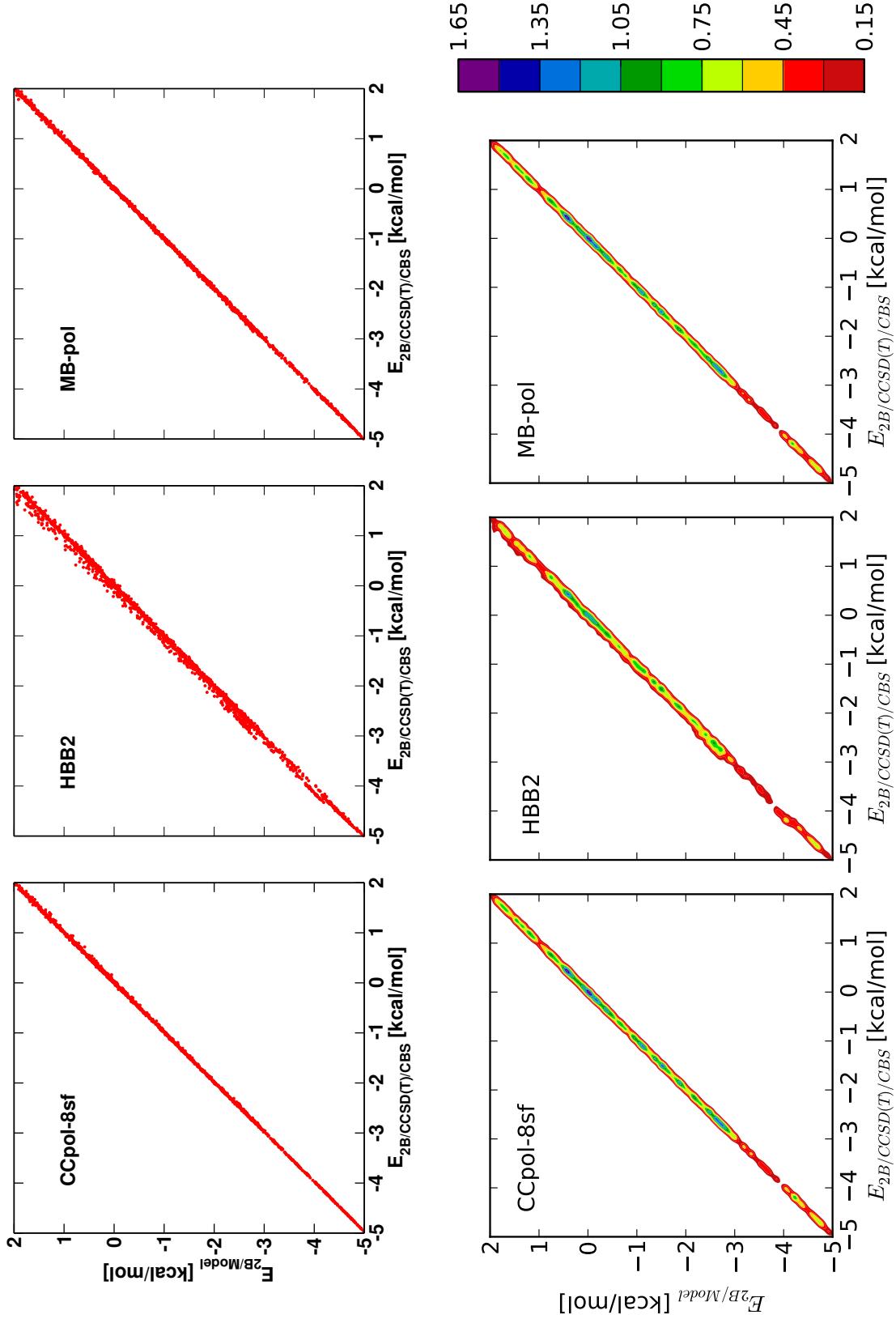


Figure S1: Two-body interaction energies for the water dimers from the `ts-ccpol.xyz` file.

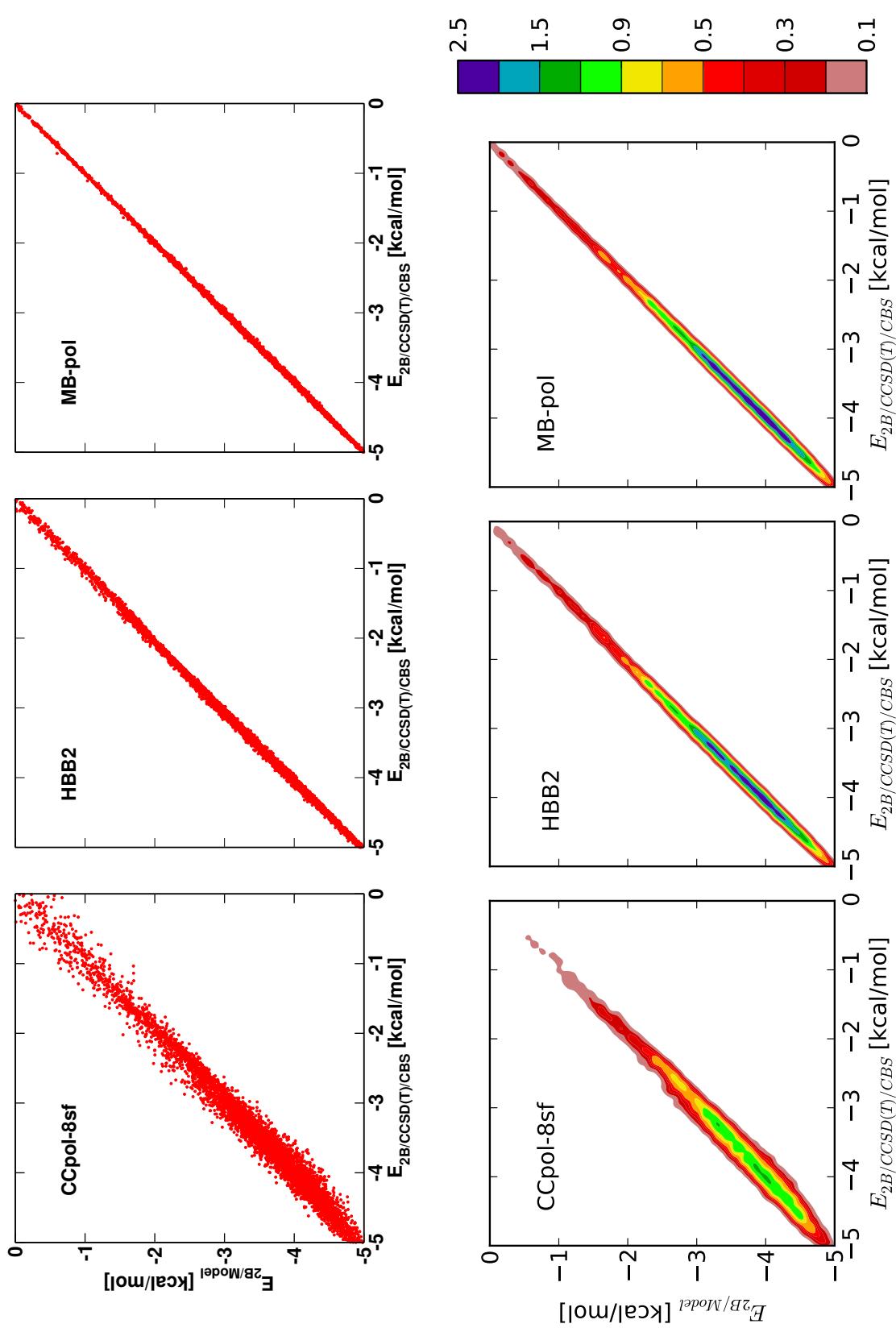


Figure S2: Two-body interaction energies for the water dimers from the ts-stationary.xyz file.

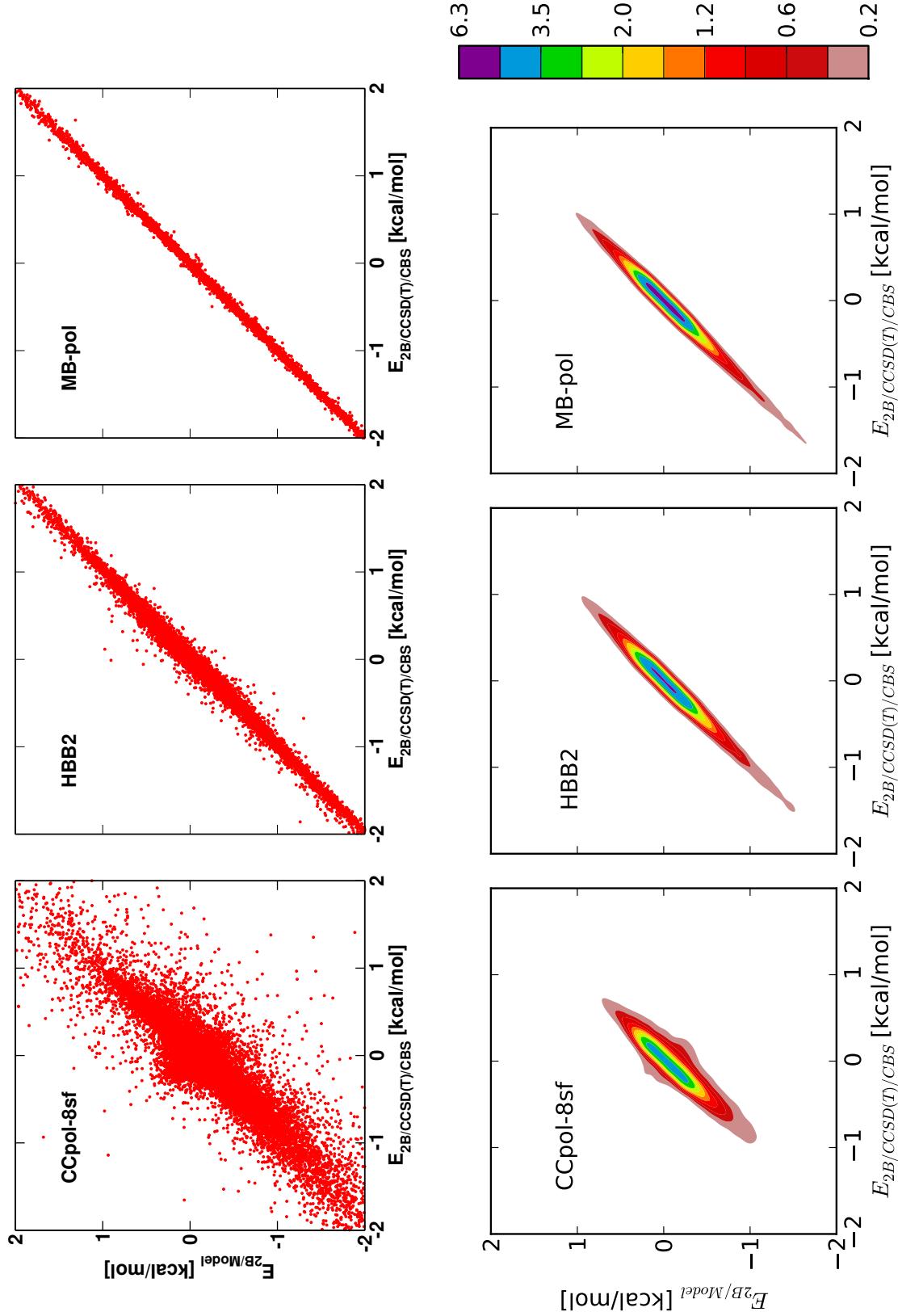


Figure S3: Two-body interaction energies for the water dimers from the `ts-pimd-run105.xyz` file.

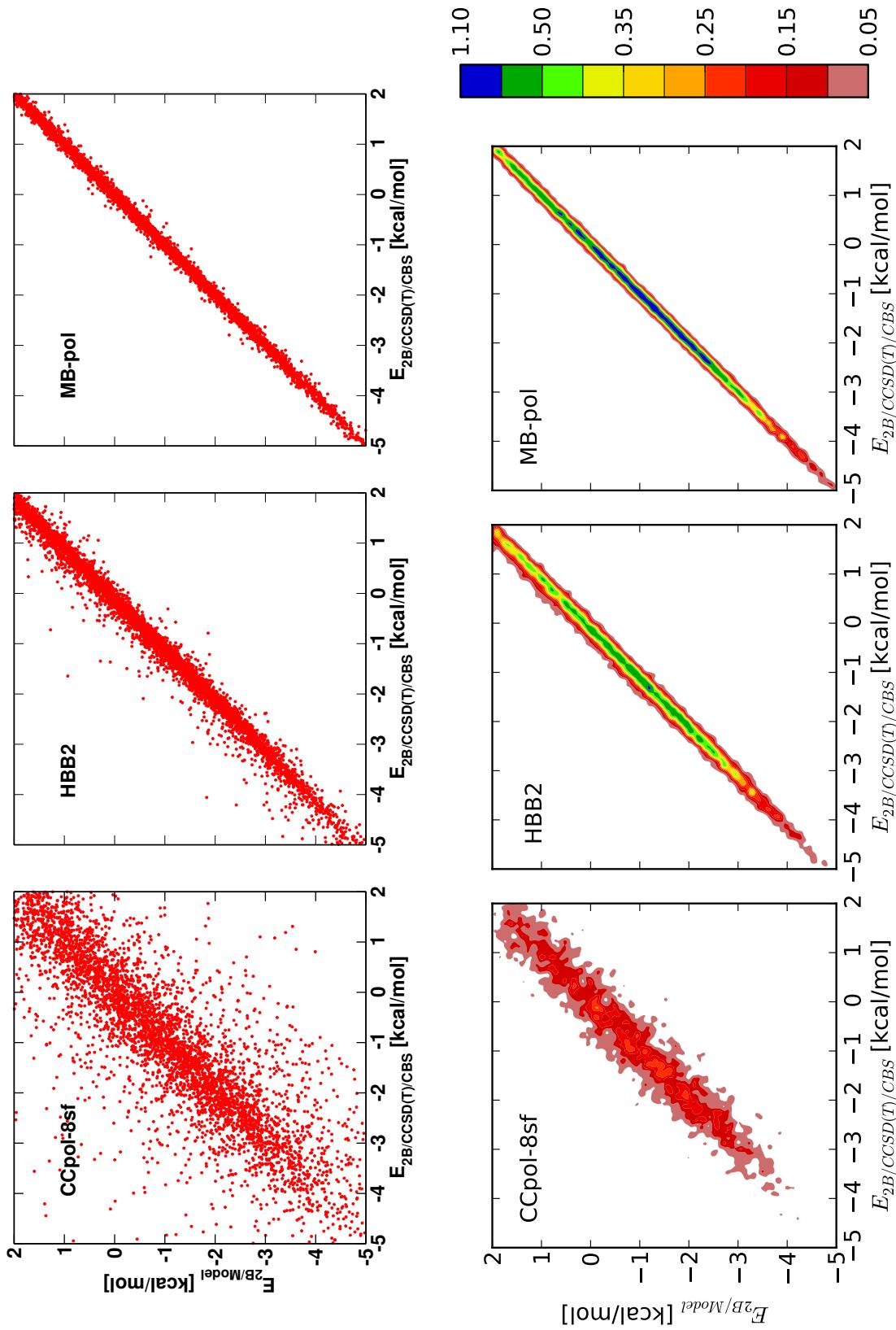


Figure S4: Two-body interaction energies for the water dimers from the `ts-pimd-run107.xyz` file.