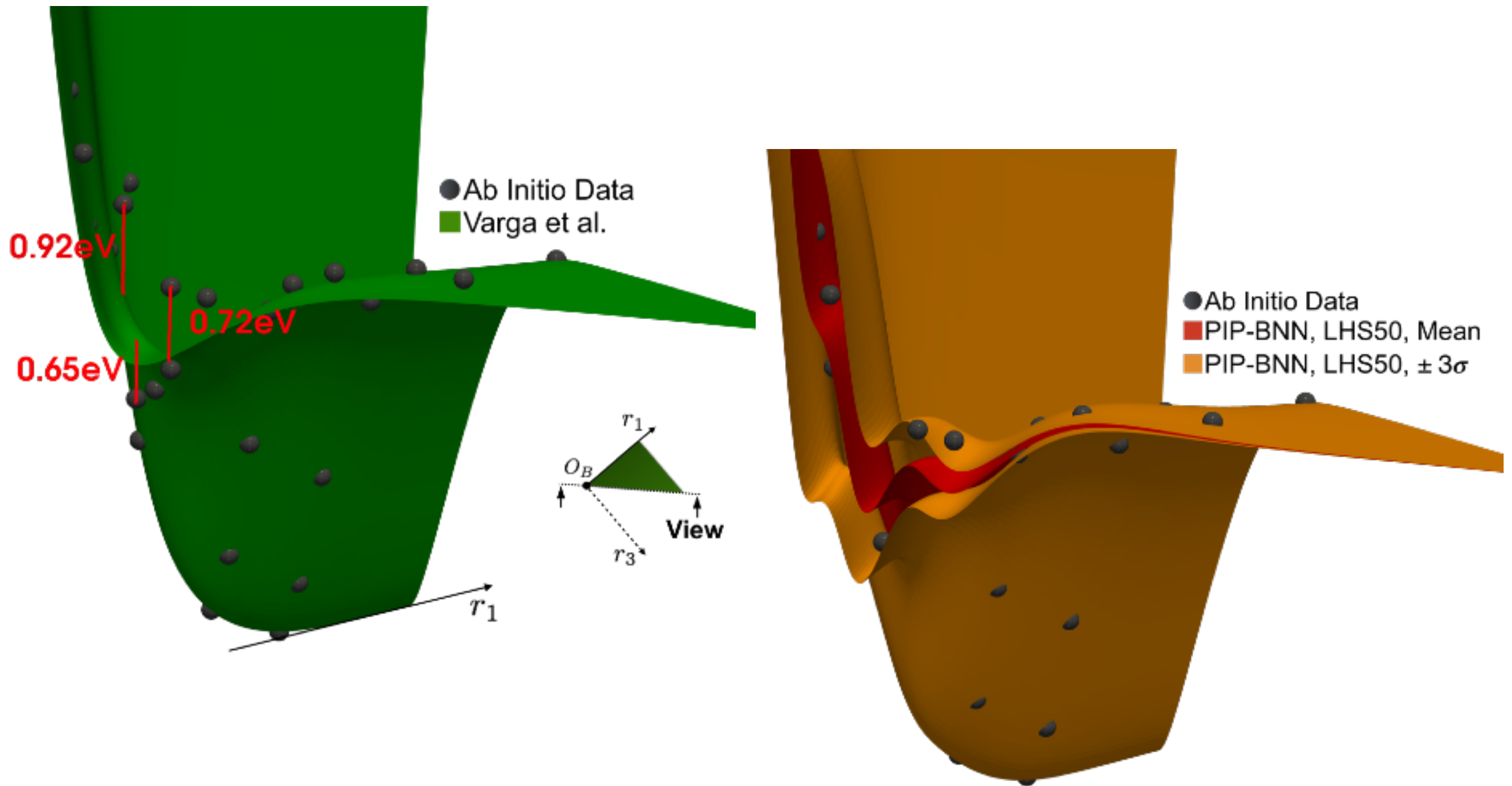


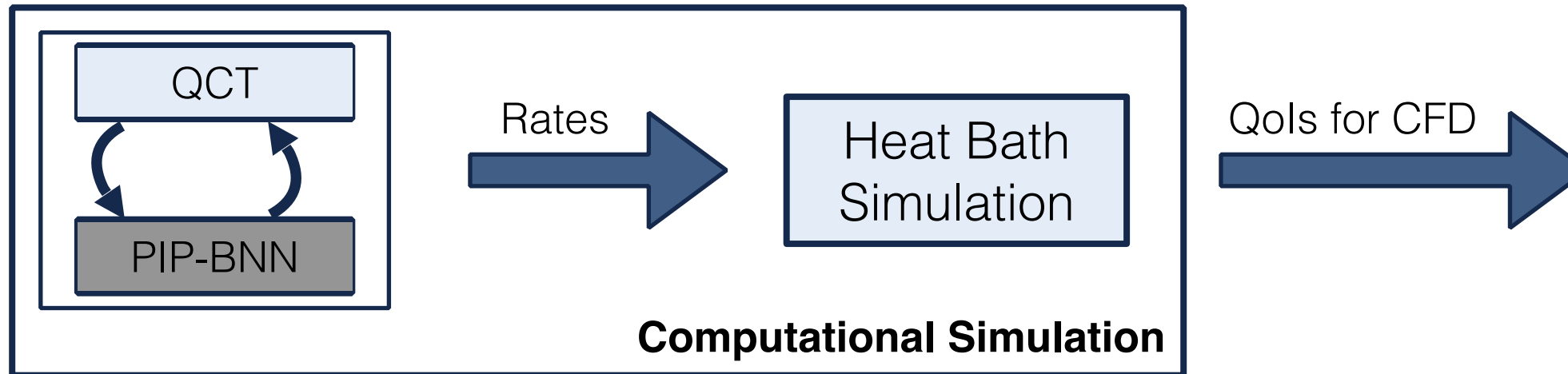
Results

3D views of the PESs at $O_A O_B O_C = 50^\circ$ for $r_1 > r_3$, compared to the correspondent ab initio data points (black dots). The green surface represents the original fit, the red one identifies the mean of the 50 PIP-BNN samples, while the orange ones correspond to the bounds of the 3-sigma confidence intervals generated by such samples.



Significant discrepancies in the exchange regions and in the repulsive wall.

Results



The PESs have been used for computing rates, that have then been employed in a Master Equation study of heat baths at fixed translational temperatures (for the plot on the right, $T_{\text{Tran}} = 10,000\text{K}$).

The PIP-BNN 99.99% confidence interval spans an interval of $\pm 45\%$ the expected value, and it does not contain the predictions from the original fit

