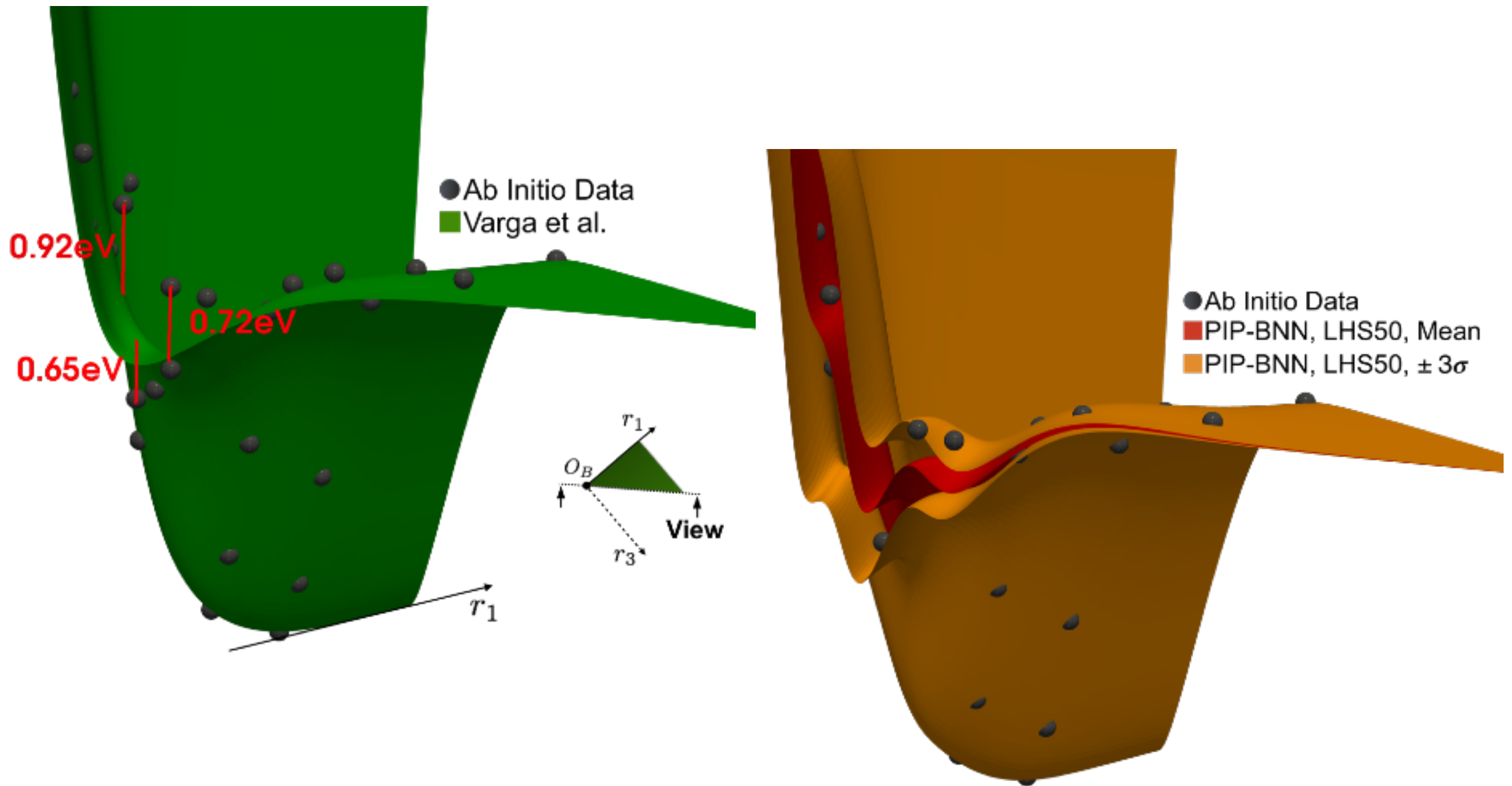


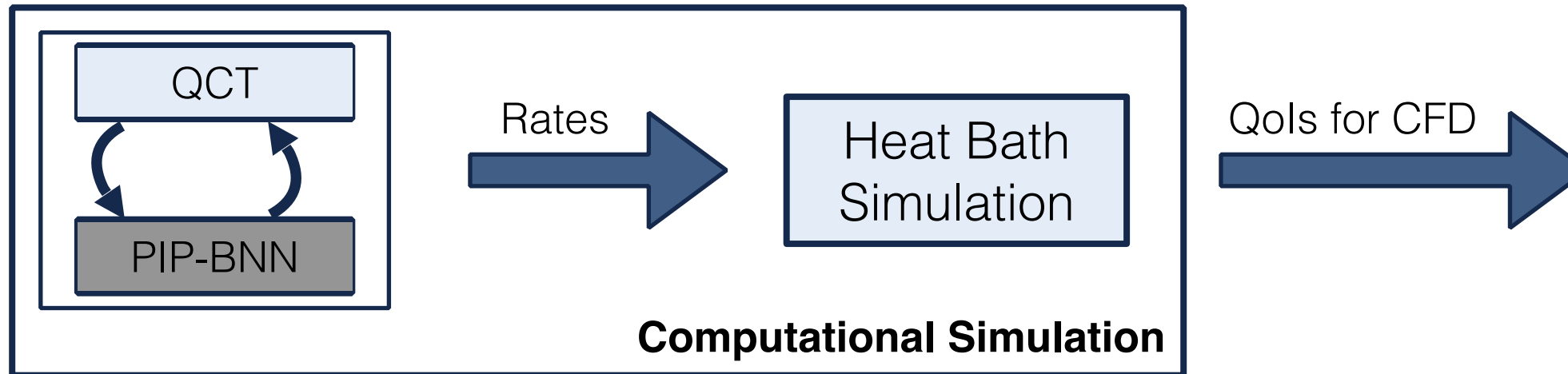
# Results

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**

