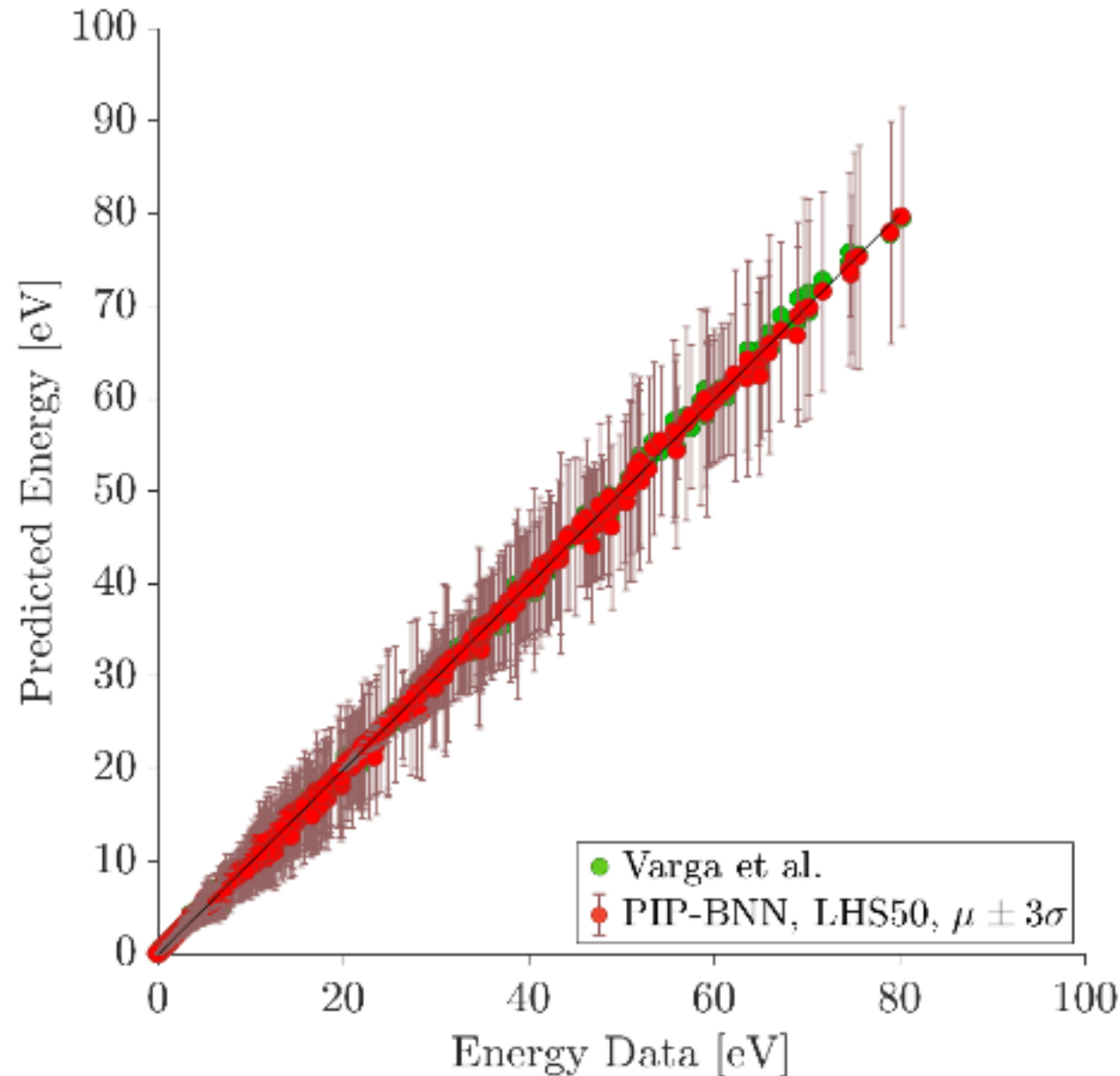
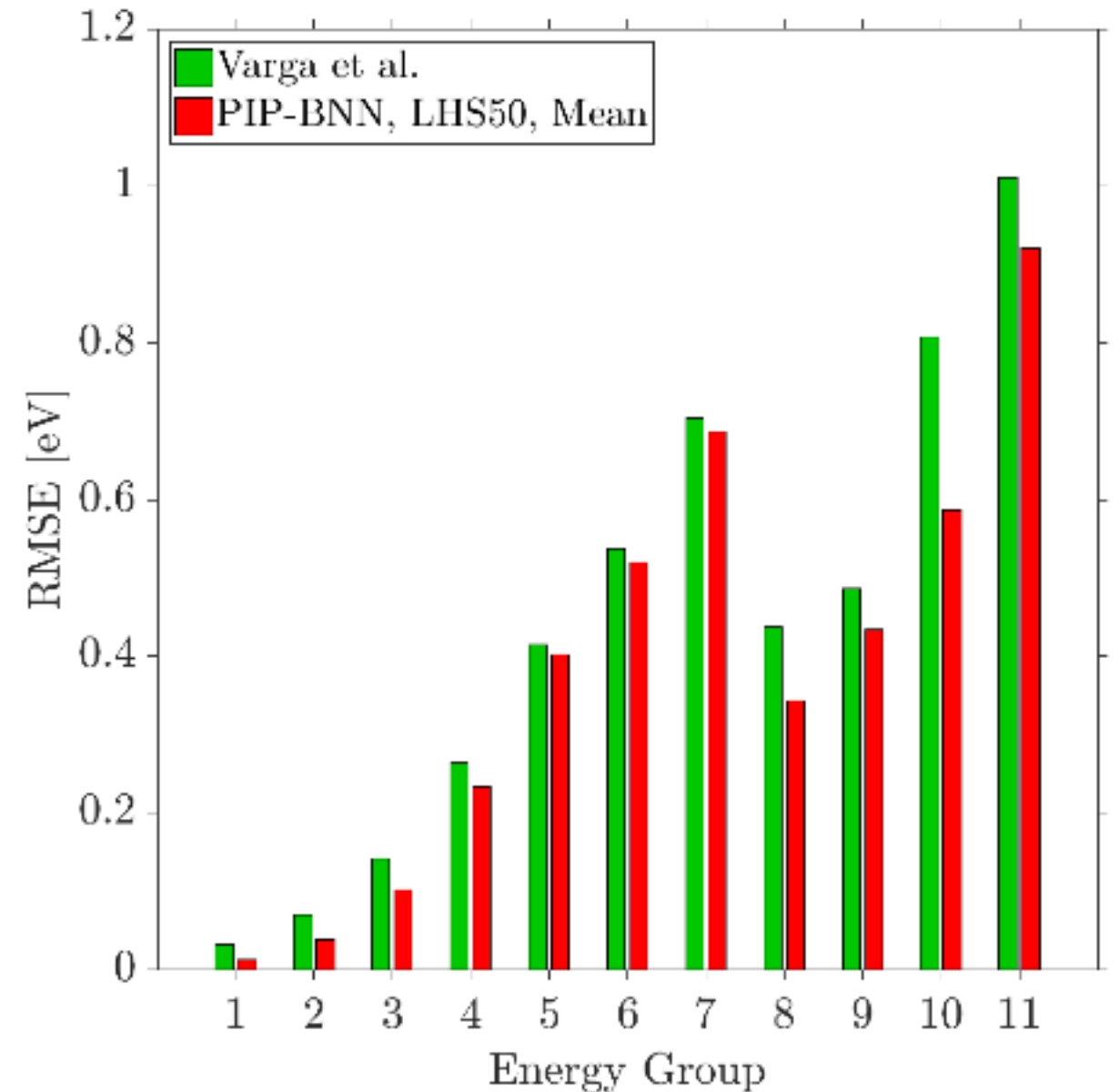


Results

As test cases, we selected 2 of the 9 O₂+O PESs developed by Varga et al. We used their same data points (~ 1600 configurations and ab initio energies), and we solved the Inverse problem. Plotted here are the results for one of the quintet PESs (with degeneracy 5/27).



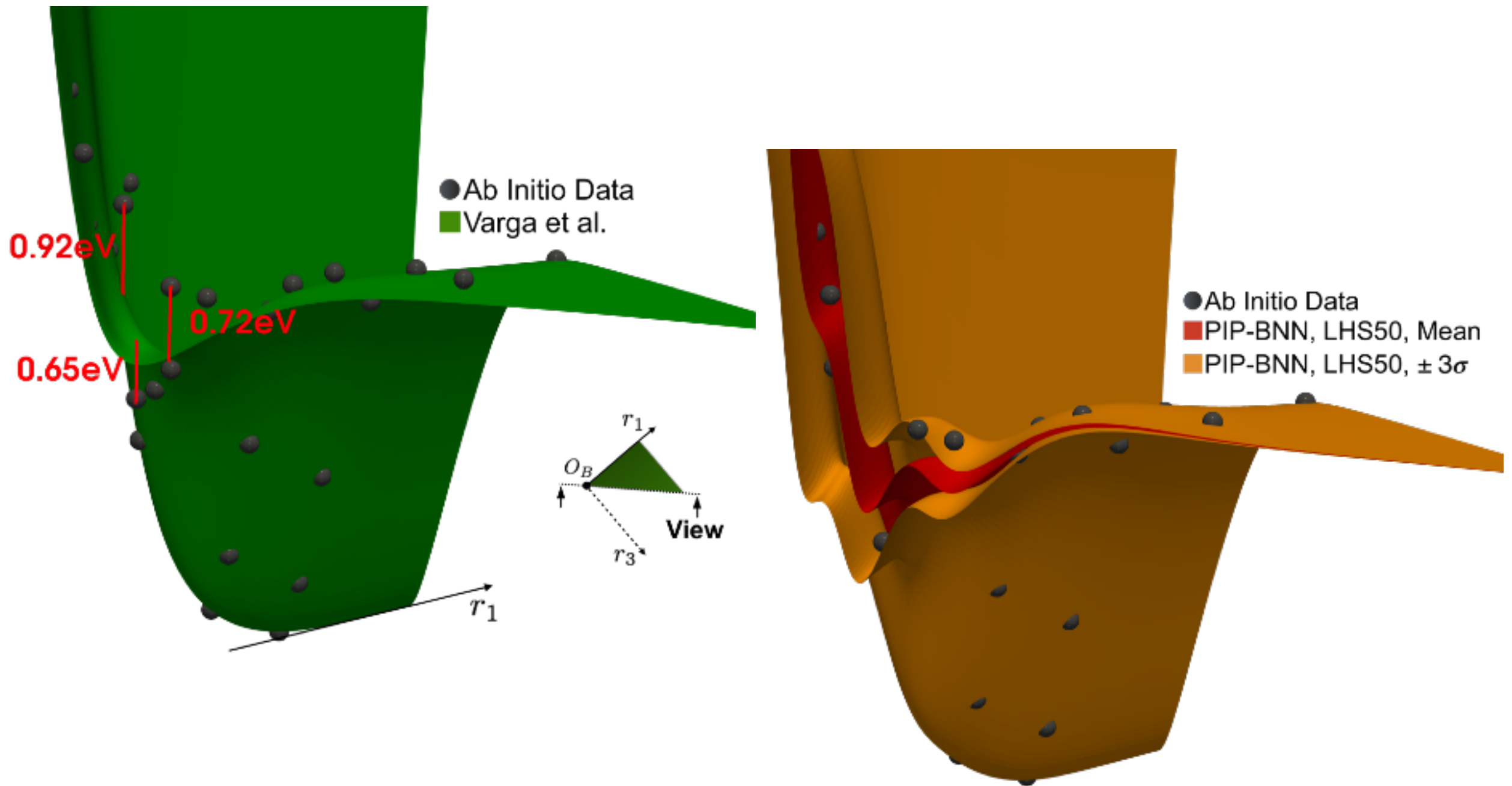
Means (red dots) and three-sigma confidence intervals (red lines) of the potential energies computed at the 1617 data points using the 50 PIP-BNN samples, compared to the energies resulting from Varga et al.'s fits (green dots).



In green, the errors produced by Varga et al.'s fits; in red, the ones generated by the means of 50 PIP-BNN samples. Upper bounds of the groups: VMax = {2:0; 4:0; 6:0; 8:0; 10:0; 15:0; 20:0; 25:0; 30:0; 50:0; 100:0} eV.

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.