The PIP-BNN Potential Energy Surface has been implemented in I-VVTC QCT Code.

QCT

PIP-BNN

Rates

19

From Deterministic To Stochastic

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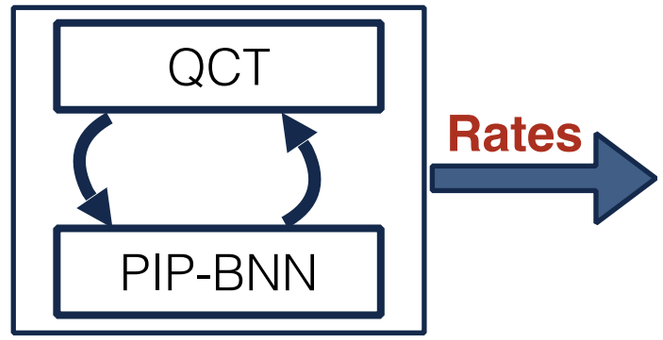
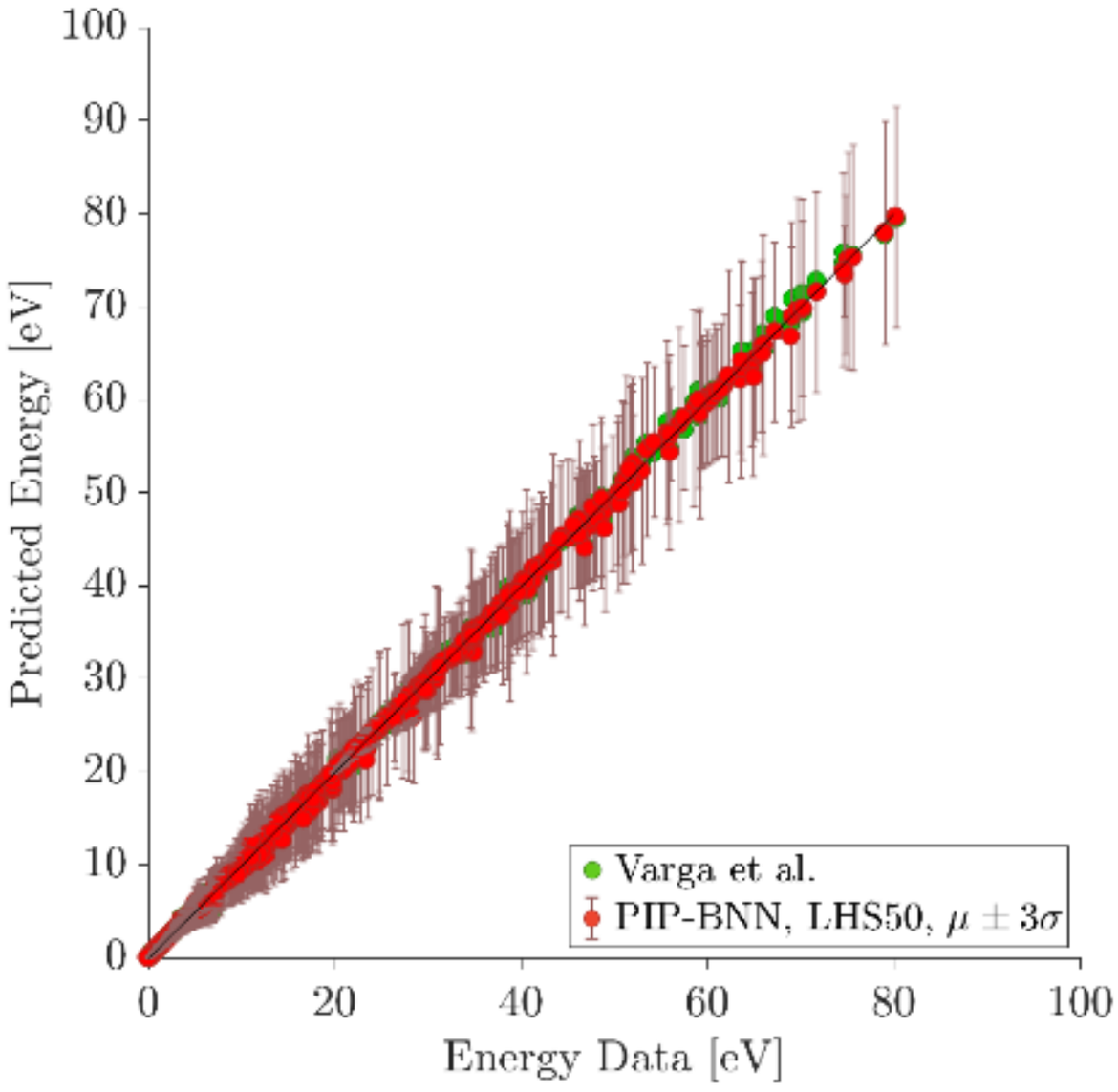
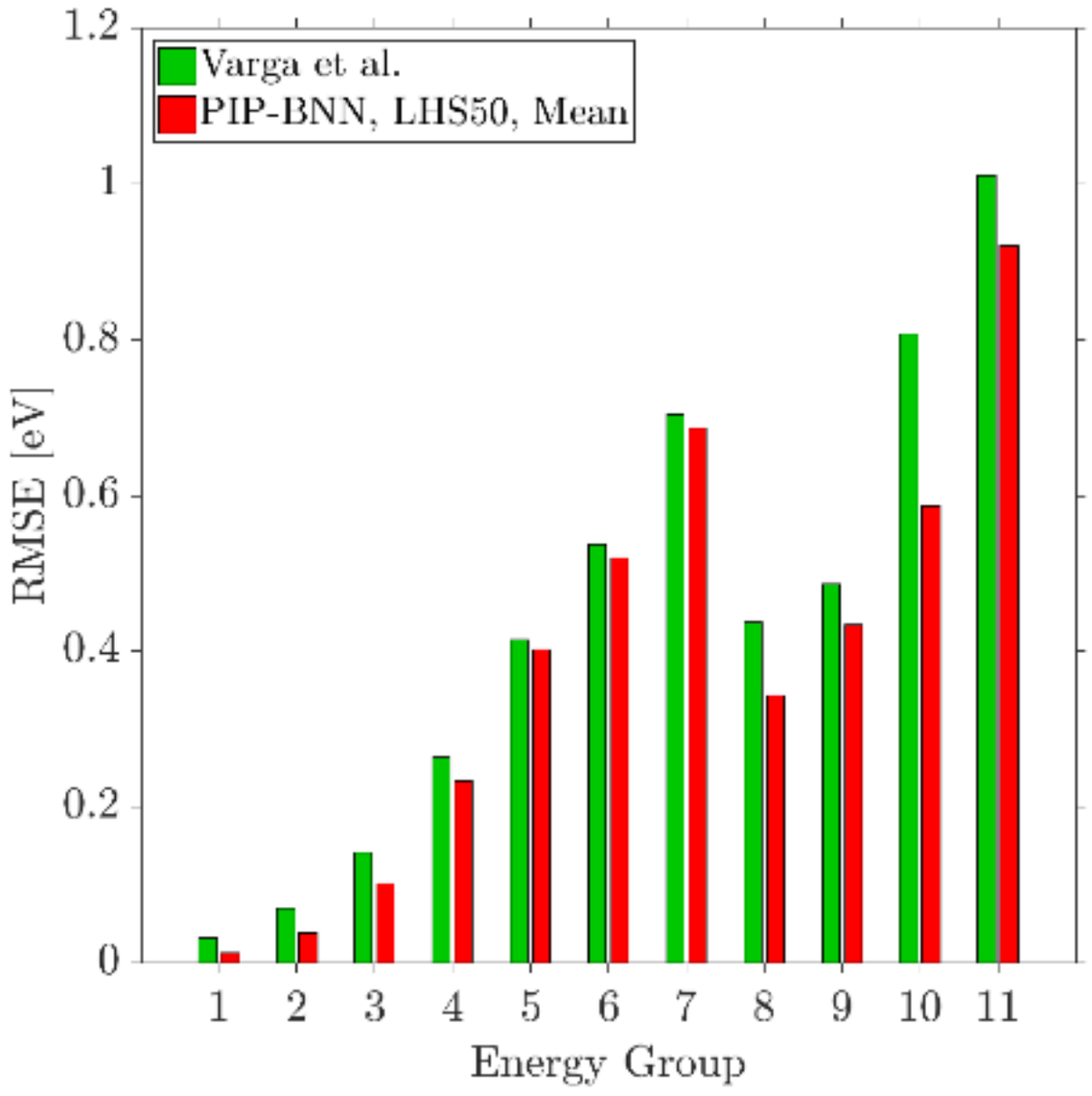


Results

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.