Supporting Information

Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost

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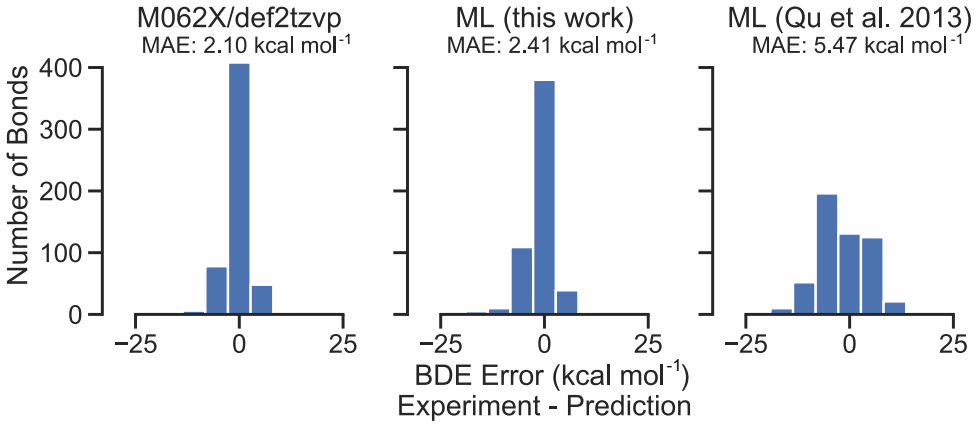
Supplementary Figures



Supplementary Figure 1: Comparison against previous BDE prediction methods. DFT calculations and predictions from the ALFABET model are compared against those using the Neural Network model of Qu *et al.* 2013.[28]

Supplementary Tables

Supplementary Table 1: Calculated Enthalpies for Error Analysis Calculations (Figure 4). All enthalpies are in Hartrees.

	Molecule	Radical	ΔH_f (mol, DFT)	ΔH_f (mol, G4)	ΔH_f (rad, DFT)	ΔH_f (rad, G4)
A	O=C1CCCC/C1=C/O	[O]/C=C1/CCCCC1=O	-423.02388	1a: -423.002035 1b: -422.983174	-422.37628	2dot: -422.358274
B	C/C=C(C)/C=C\C(=O)OC	C/C=C(C)/C=C\C([O])=O	-462.2693	cis-3: -462.256891 trans-3: -462.264775	-422.39872	cis-4dot: -462.264775 trans-4dot: -422.328661
C	NC(=O)CCN(N)C(=O)O	NC(=O)CCN(N)C([O])=O	-547.63572	5: -547.576587	-546.99392	6dot: -546.958135 *(includes CO_2)*
D	Nc1cc(N)cc(O)c1	Nc1cc(N)cc([O])c1	-418.03083	7: -417.999734	-417.36249	8dot: -417.363114