

QM/MM Investigation of Second Coordination Shell Residues in [NiFe]-Hydrogenases

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Supporting Information

Detailed analysis of MM and QM contributions to the QM/MM energies.

Note: MM energy is the same in all single point calculations.

Table RS1. QM and MM energies of H₂ heterolytic splitting by EH1.

Proton acceptor	BP86		BP86-D3	B3LYP-D3	TPSSH-D3
	QM	MM	QM	QM	QM
Arginine 509 ⁺	17.2	2.1	14.1	11.8	13.0
Cysteine 76	3.1	-6.8	4.6	-3.1	-0.4
Cysteine 576	-10.9	2.5	-9.5	-17.8	-14.7

Table RS2. QM and MM energies of H₂ heterolytic splitting by K-EH1.

Proton acceptor	BP86		BP86-D3	B3LYP-D3	TPSSH-D3
	QM	MM	QM	QM	QM
Cysteine 76	10.5	-22.4	10.6	3.3	6.2
Cysteine 576	-13.3	3.2	-12.6	-20.5	-17.6