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MDPI

Theoretical studies of a Silica-Functionalized Polyacrylamide for Calcium Scale Inhibition

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Table S1. The DFT calculated energy values and binding energies of the studied complexes.

Name	Energy (Hatrees)	Binding Energy (Hatrees)	Binding Energy(kJ/mol)
Ca	-677.466		
AA_AA_AA_AM	-1050.32		
AA_AA_AM_AM	-1030.43		
AA_AM_AM_AM	-1010.54		
Pure_PAM	-951.366		
PAM_hydro	-1029.12		
PAM_SiO2	-1580.54		
Complexes			
Ca_AA_AA_AA_AM	-1726.47	1.308	820.463
Ca_AA_AA_AM_AM	-1707.05	0.846	530.815
Ca_AA_AM_AM_AM	-1687.73	0.282	177.096
Ca_Pure_PAM	-1629.00	**-0.169**	**-106.051**
Ca_PAM_hydro	-1707.05	**-0.461**	**-289.027**
Ca_PAM_SiO2	-2258.45	**-0.439**	**-275.301**
Ca_PAM_SiO2b	-2258.51	**-0.499**	**-313.431**