Supplementary information for "Adsorption of alcohols and hydrocarbons on nonstoichiometric cementite {010} surfaces."

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We show in Figures 1-9 other local minima found in our simulations for several molecules adsorbed over nonstoichiometric cementite {010}. These configurations are higher in energy than the configurations shown in the main paper. Tables I and II show the adsorption energies corresponding to the local minima pictured in this document.

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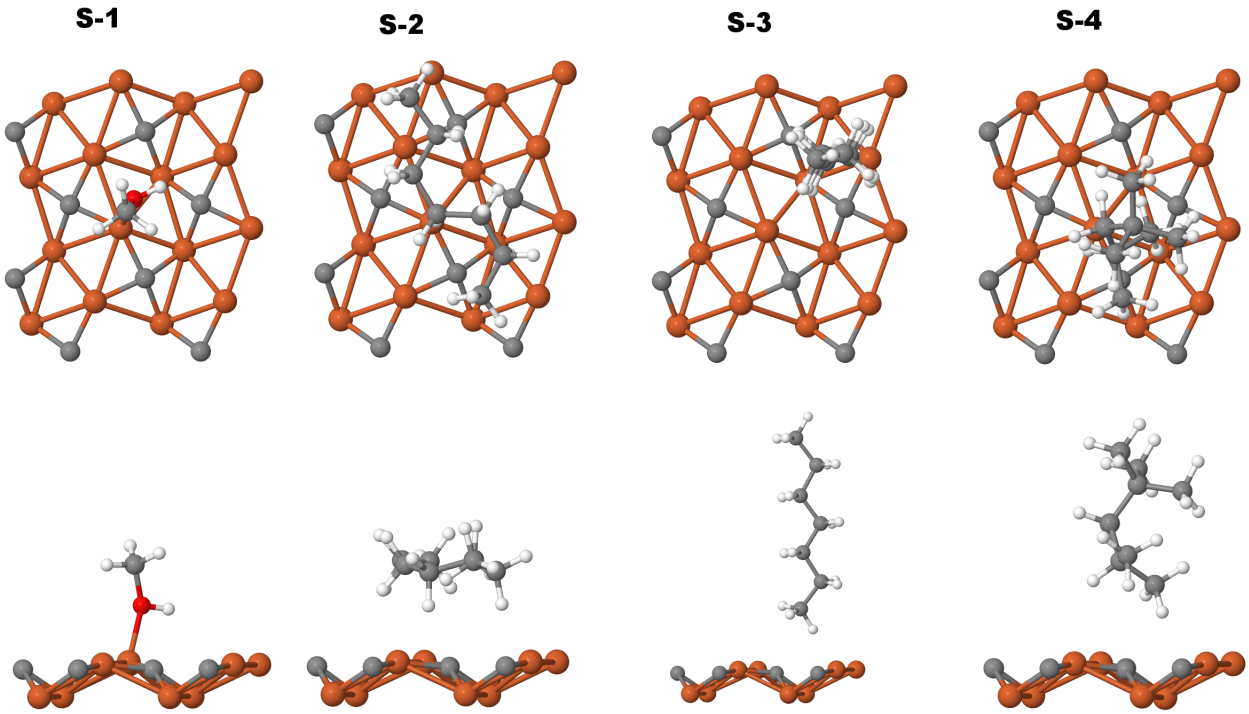

FIG. 1: Detail of the local minima found for the adsorption of noncyclic hydrocarbons on nonstoichiometric cementite {010}. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

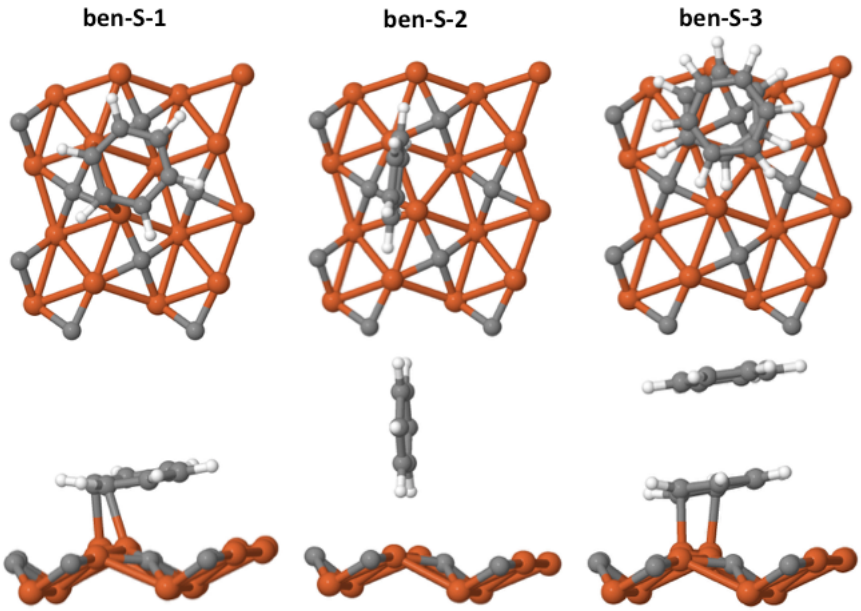

FIG. 2: Detail of the local minima found for the adsorption of benzene on nonstoichiometric cementite {010}. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

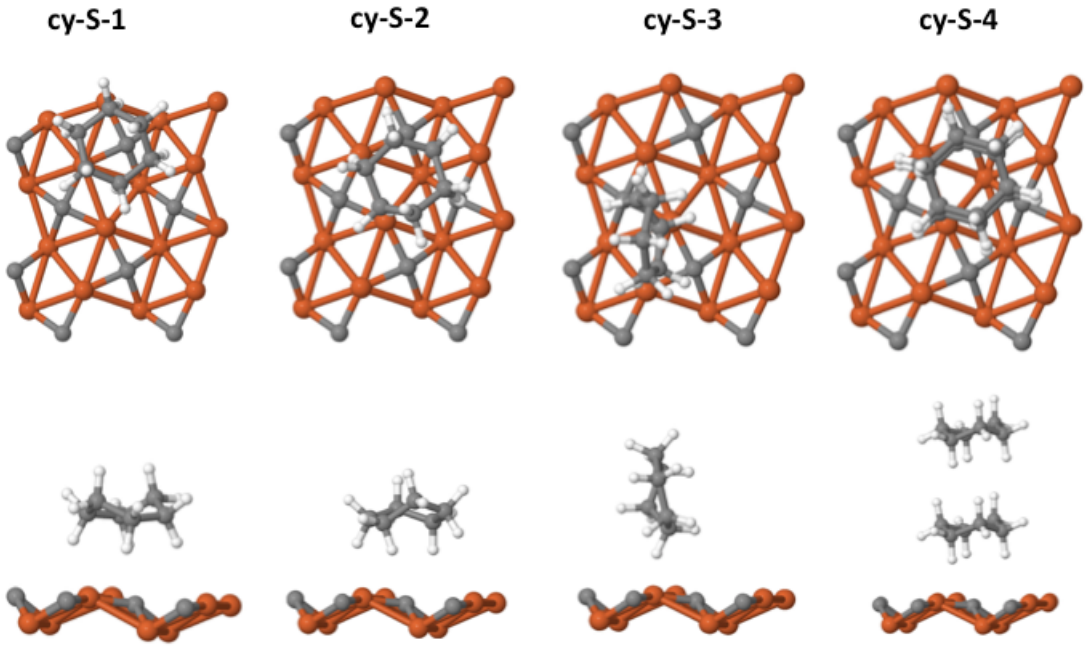

FIG. 3: Detail of the local minima found for the adsorption of cyclohexane on nonstoichiometric cementite {010}. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

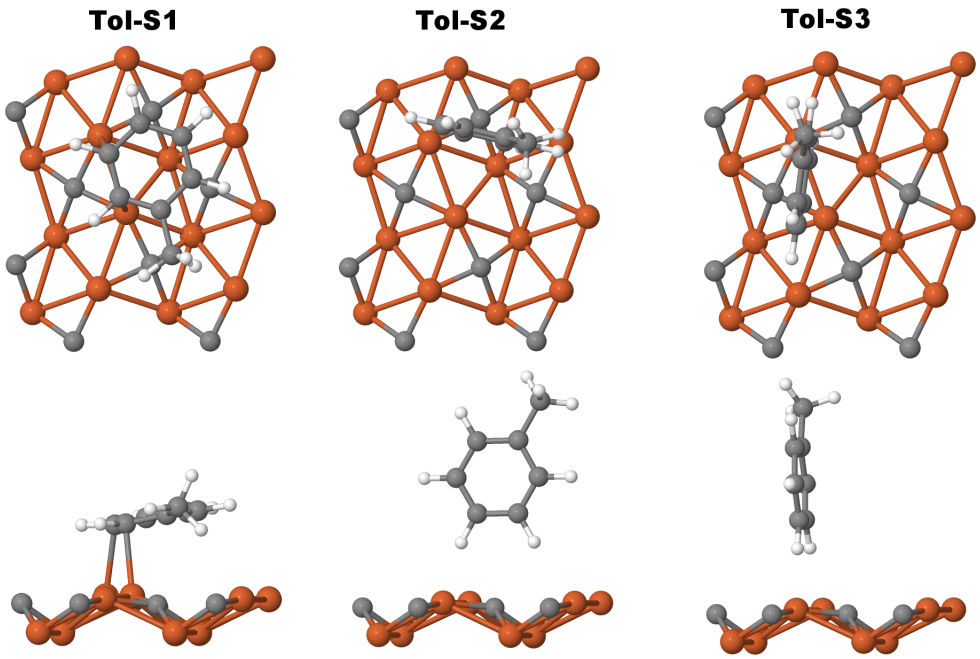

FIG. 4: Detail of the local minima found for the adsorption of toluene on nonstoichiometric cementite {010} at low coverage. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

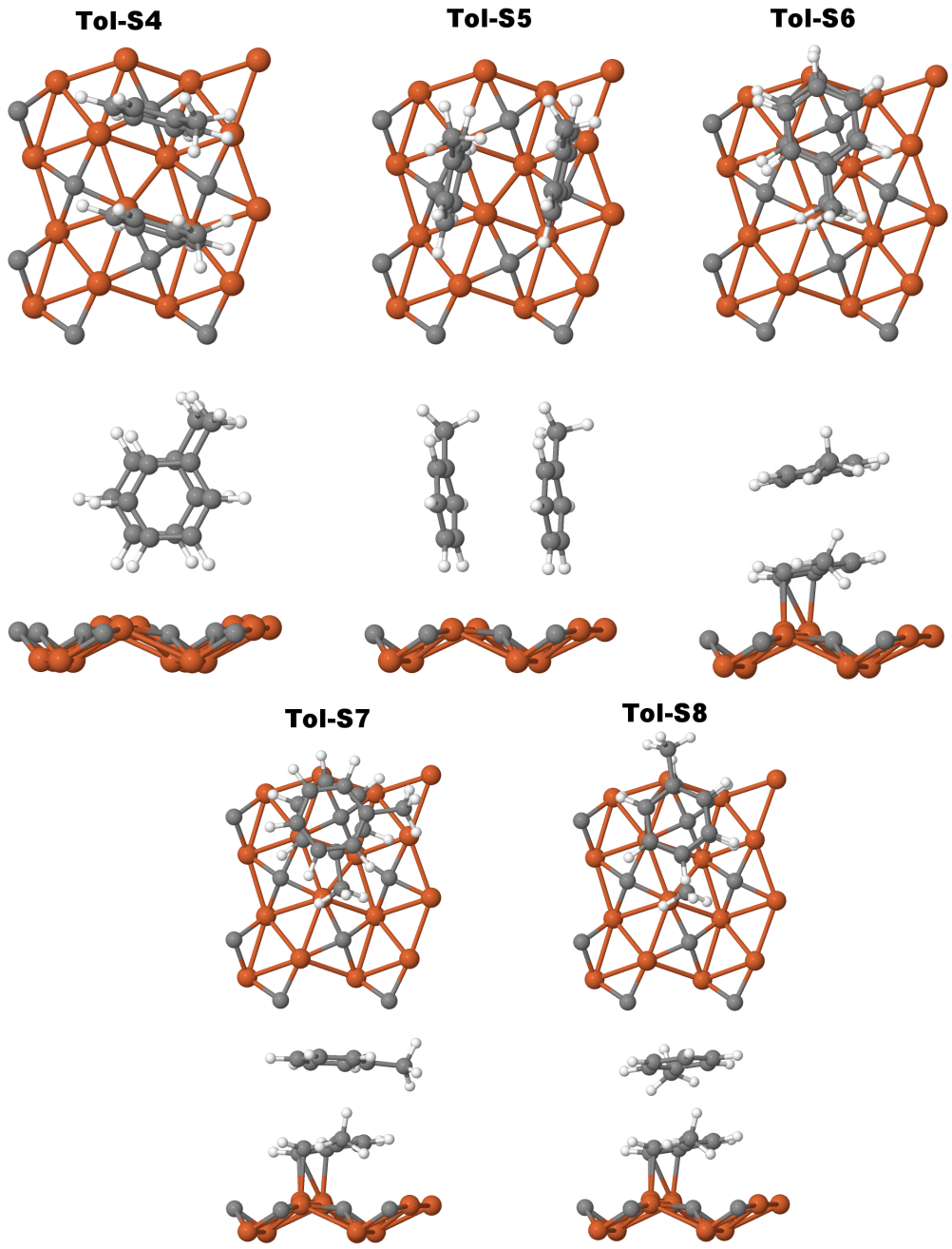

FIG. 5: Detail of the local minima found for the adsorption of toluene on nonstoichiometric cementite {010} at high coverage. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

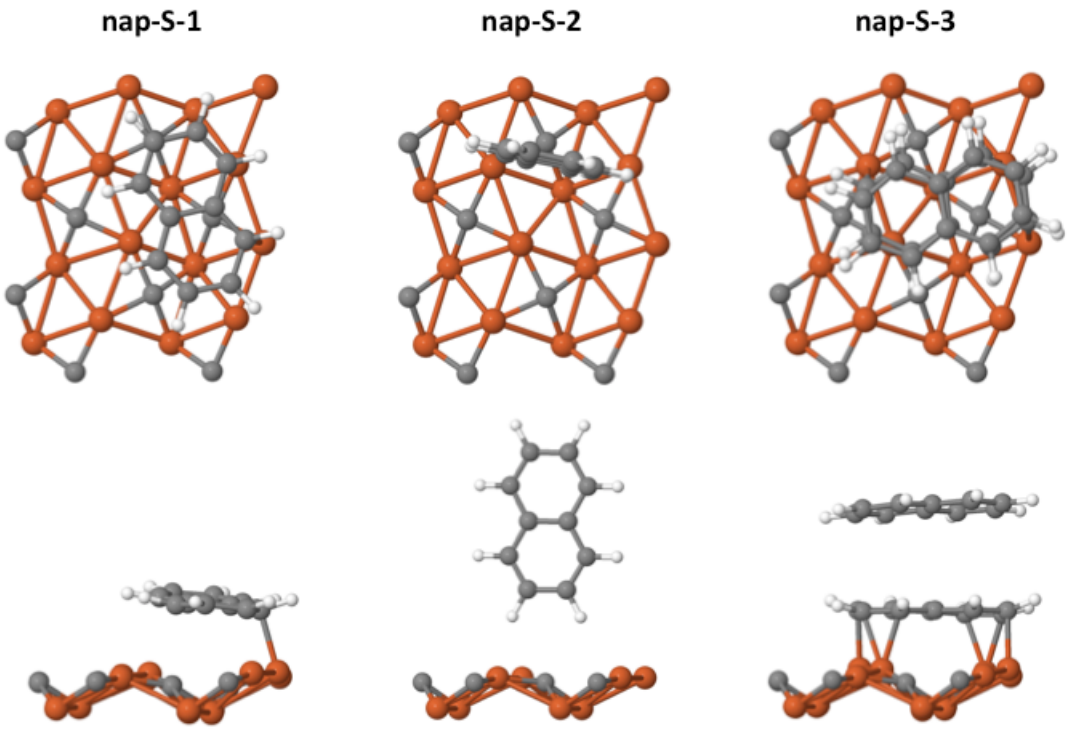

FIG. 6: Detail of the local minima found for the adsorption of naphthalene on nonstoichiometric cementite {010}. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

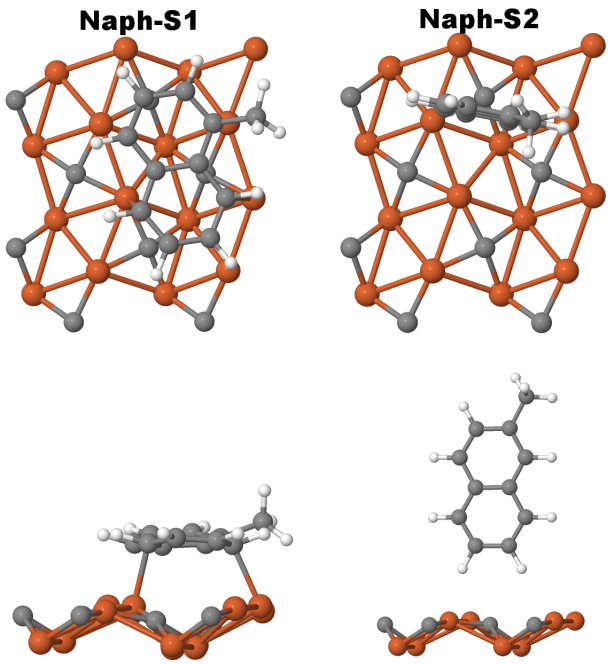

FIG. 7: Detail of the local minima found for the adsorption of 1-methylnaphthalene on nonstoichiometric cementite {010} at low coverage. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

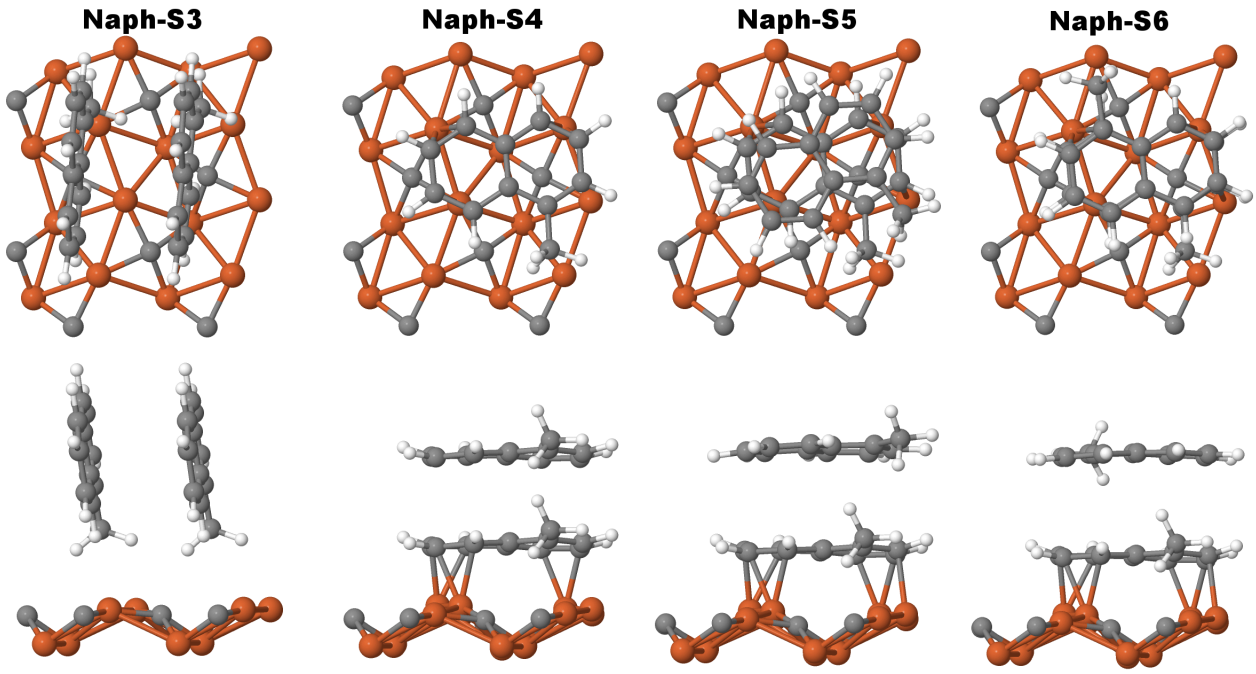

FIG. 8: Detail of the local minima found for the adsorption of 1-methylnaphthalene on nonstoichiometric cementite {010} at high coverage. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

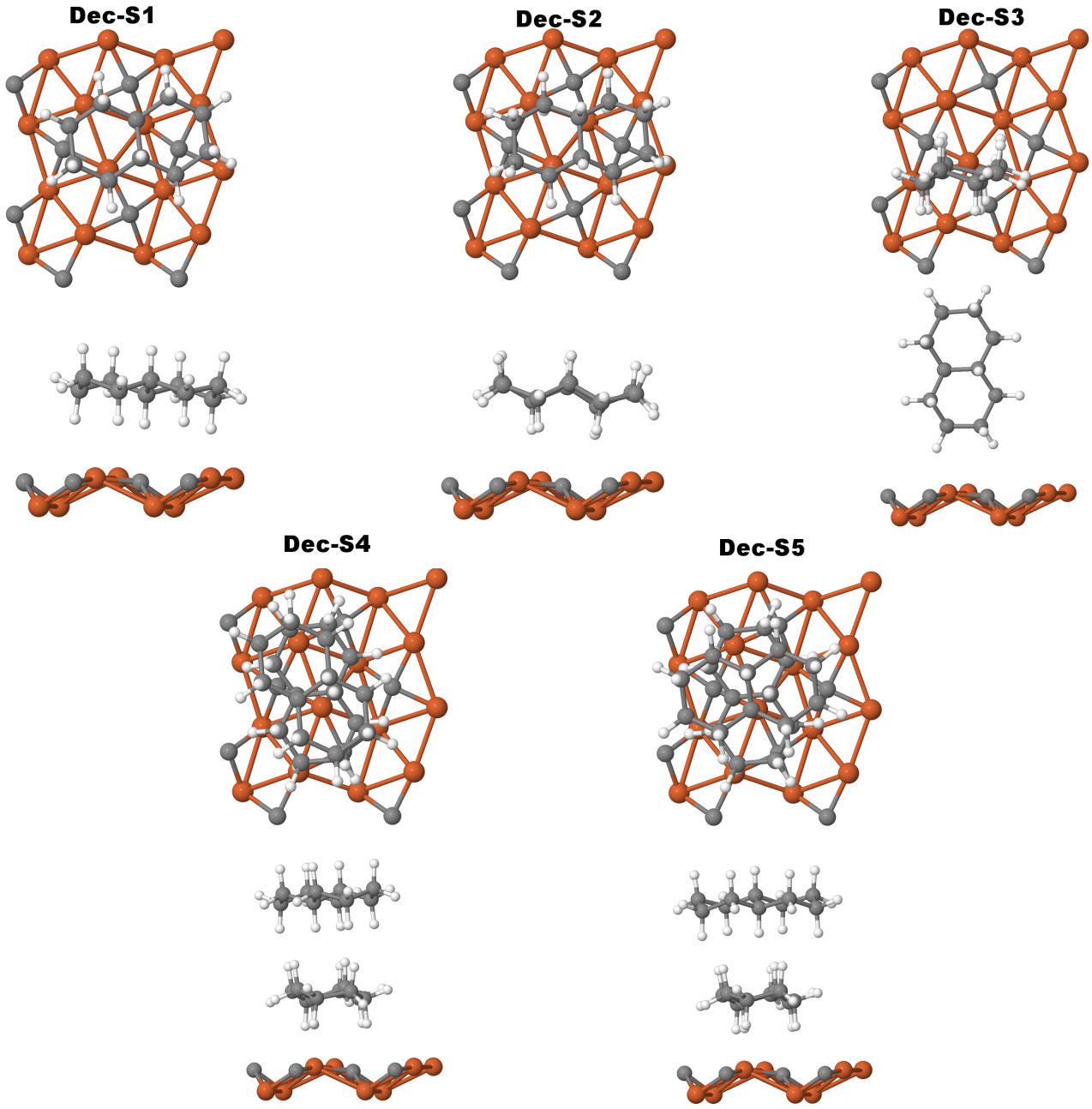

FIG. 9: Detail of the local minima found for the adsorption of decalin on nonstoichiometric cementite {010}. For each configuration, the top picture shows the view from the top, and the bottom picture shows a side view.

TABLE I: Adsorption energies for the local minima found for the nonaromatic organic molecules considered in this study. All energies are given in eV.

Configuration	Adsorption energy
Methanol	
S-1	-0.97
n-heptane	
S-2	-1.51
S-3	-0.61
Isooctane	
S-4	-0.64
Cyclohexane	
Cy-S1	-1.08
Cy-S2	-1.35
Cy-S3	-0.42
Cy-S4	-1.52
Decalin	
Dec-S1	-2.03
Dec-S2	-2.09
Dec-S3	-0.89
Dec-S4	-2.75
Dec-S5	-2.78

TABLE II: Adsorption energies for the local minima found for the aromatic organic molecules considered in this study. All energies are given in eV.

Configuration	Adsorption energy
Benzene	
Ben-S1	-1.74
Ben-S2	-0.53
Ben-S3	-2.36
Toluene	
Tol-S1	-1.83
Tol-S2	-0.66
Tol-S3	-0.62
Tol-S4	-1.59
Tol-S5	-1.63
Tol-S6	-2.70
Tol-S7	-2.74
Tol-S8	-2.71
naphthalene	
Nap-S1	-2.44
Nap-S2	-0.65
Nap-S3	-4.10
1-methylnaphthalene	
Naph-S1	-2.43
Naph-S2	-0.76
Naph-S3	-2.61
Naph-S4	-4.36
Naph-S5	-4.40
Naph-S6	-4.40