Supplementary Information for

Theoretical Exploration of Properties of Iron–Silicon Interface Constructed by Depositing Fe on Si(111)-(7×7)

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Table S1. The total energy ($E_{n\text{Fe/DASF}}$) and the averaged binding energy ($E_{\text{b\_ave}}$) for the "**S*n***" models with all the Fe atoms on the DASF surface, where n is the number of Fe atoms.

Model "**S*n***"	$E_{n\text{Fe/DASF}}$ (eV)	$E_{\text{b\_ave}}$ (eV)
S1	−1736.387769	−4.228
S2	−1744.376335	−4.409
S3	−1752.730515	−4.591
S4	−1760.970227	−4.654
S5	−1769.236751	−4.697
S6	−1778.445066	−4.882
S7	−1787.772033	−5.032
S8	−1795.566334	−4.952
S9	−1803.727181	−4.931
S10	−1812.424595	−4.968
S11	−1820.143884	−4.909
S12	−1828.500031	−4.913
S13	−1836.407191	−4.882
S14	−1843.877881	−4.824
S15	−1851.878756	−4.810
S16	−1859.300691	−4.760
S17	−1866.934091	−4.729

Table S2. The total energy ($E_{n\text{Fe/DASF}}$) and the averaged binding energy ($E_{\text{b\_ave}}$) for the "**Fe*n***" models with Fe permeation on the DASF surface, where n is the number of Fe atoms.

Model "**Fe*n***"	$E_{n\text{Fe/DASF}}$ (eV)	$E_{\text{b\_ave}}$ (eV)
Fe1	−1736.919476	−4.760
Fe2	−1744.916874	−4.680
Fe3	−1753.349987	−4.798
Fe4	−1761.495353	−4.785
Fe5	−1769.542338	−4.758
Fe6	−1778.445066	−4.882
Fe7	−1787.772033	−5.032
Fe8	−1796.452239	−5.063
Fe9	−1805.041663	−5.077
Fe10	−1813.612284	−5.087
Fe11	−1821.572245	−5.039
Fe12	−1829.706616	−5.014
Fe13	−1838.012209	−5.006
Fe14	−1846.051198	−4.980
Fe15	−1854.437957	−4.980
Fe16	−1862.433833	−4.956
Fe17	−1870.187944	−4.921
Fe18	−1879.063258	−4.952
Fe19	−1887.699004	−4.967
Fe25	−1935.001270	−4.851
Fe28	−1960.836422	−4.890
Fe31	−1985.325913	−4.878
Fe35	−2016.117906	−4.812
Fe39	−2047.713526	−4.780