

Supplementary Data

Supplementary Data 1: Optimized SiH^{δ-}-ZVI in VASP for electronic structure calculations

SiH^{δ-}-ZVI

1.0000000000000000

14.823999999999998 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.823999999999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.458800000000001

Fe O Si H Na

175 53 1 2 1

Selective dynamics

Direct

0.9931899999999985 0.0069299999999970 0.0301899999999975 F F F

0.9957300000000018 0.0049599999999970 0.1257499999999965 F F F

0.9941299999999984 0.9936199999999999 0.2346300000000028 F F F

0.1122900000000016 0.1005499999999984 0.0827600000000004 F F F

0.1016100000000009 0.0873899999999992 0.1803499999999971 F F F

0.2098999999999975 0.0060900000000004 0.0298999999999978 F F F

0.2085500000000025 0.0025600000000026 0.1257299999999972 F F F

0.2088999999999999 0.0047300000000021 0.2346799999999973 F F F

0.3043800000000019 0.0915099999999995 0.0826599999999971 F F F

0.2936499999999995 0.0890600000000035 0.1799999999999997 F F F

0.3994399999999985 0.9940199999999990 0.0295800000000028 F F F

0.4007999999999967 0.0048699999999968 0.1259000000000015 F F F

0.3990500000000026 0.9928799999999995 0.2342200000000005 F F F

0.5191400000000002 0.1002300000000034 0.0767299999999977 F F F

0.5071099999999973 0.0867500000000021 0.1743900000000025 F F F

0.6169900000000013 0.9930999999999983 0.0284300000000002 F F F

0.6140299999999996 0.0032599999999974 0.1241600000000034 F F F

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0.70902999999999985	0.10081999999999988	0.07741999999999965	F	F	F
0.69749000000000019	0.08849000000000002	0.17522999999999991	F	F	F
0.80532999999999979	0.99210999999999967	0.03721000000000017	F	F	F
0.80469999999999969	0.00504999999999971	0.13152000000000019	F	F	F
0.80299999999999973	0.99419000000000032	0.22955999999999993	F	F	F
0.89829000000000029	0.10168999999999978	0.08306000000000032	F	F	F
0.91080999999999979	0.10056999999999976	0.18028999999999994	F	F	F
0.99510000000000008	0.19536999999999969	0.03735000000000035	F	F	F
0.00726000000000023	0.19615000000000029	0.13264000000000021	F	F	F
0.00659999999999988	0.20808999999999986	0.22856999999999977	F	F	F
0.11202000000000011	0.28970000000000034	0.08301000000000016	F	F	F
0.11359000000000021	0.30355999999999974	0.18003999999999982	F	F	F
0.21020000000000004	0.19494000000000026	0.03690999999999989	F	F	F
0.19885000000000002	0.19581999999999977	0.13306000000000004	F	F	F
0.19633999999999993	0.19588000000000025	0.22870999999999995	F	F	F
0.30579000000000018	0.30107000000000028	0.07661999999999984	F	F	F
0.30362999999999983	0.30210000000000029	0.18652000000000016	F	F	F
0.39920999999999965	0.18160999999999992	0.03576999999999994	F	F	F
0.41060000000000023	0.19442000000000009	0.13121999999999990	F	F	F
0.41230000000000019	0.18173999999999978	0.22677000000000019	F	F	F
0.49654000000000031	0.28918999999999978	0.07741000000000004	F	F	F
0.49712000000000024	0.30136000000000025	0.17473999999999999	F	F	F
0.61612999999999983	0.18160000000000031	0.02210000000000018	F	F	F
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0.60125000000000003	0.18178999999999995	0.22738999999999998	F	F	F
0.70929000000000029	0.28967999999999971	0.07103000000000004	F	F	F
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0.89947000000000009	0.50334000000000015	0.17900999999999981	F	F	F

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0.3036299999999983	0.5058399999999992	0.3150300000000001	F	F	F
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0.2052419971605499	0.5964221675068531	0.3780812326205352	T	T	T
0.2910400000000024	0.6964600000000019	0.2903599999999997	F	F	F
0.3904325639132264	0.6485880747745121	0.4071339367778319	T	T	T
0.5044499999999985	0.7098599999999990	0.2978700000000032	F	F	F
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0.8853999999999971	0.7096000000000018	0.2908299999999997	F	F	F
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0.8440780809629994	0.2995371160909506	0.4040555612791392	T	T	T
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0.9868299999999977	0.6054000000000030	0.3015600000000020	F	F	F
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0.1963099999999969	0.5959000000000003	0.3013699999999986	F	F	F
0.2791627204689164	0.7104750422321008	0.3795465095549205	T	T	T
0.4047300000000007	0.6020499999999984	0.3004900000000035	F	F	F
0.4911261595939690	0.7172853937233281	0.3776726115732372	T	T	T
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0.9998199999999997	0.7960300000000018	0.3059900000000013	F	F	F
0.0825606831384455	0.8936923121238117	0.3813710095353220	T	T	T
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0.4465309457864644	0.7128476056631901	0.5599543130991360	T	T	T
0.2552061407938553	0.6370627875352937	0.5875477075774497	T	T	T