

Electronic Supplementary Information

Structural, Electronic and Magnetic Properties of Ni Nanoparticles Supported on the TiC(001) Surface

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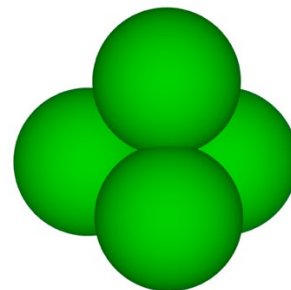
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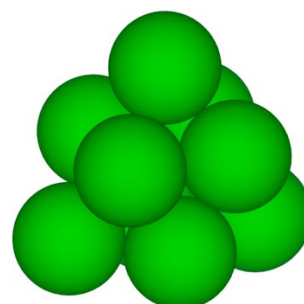
1. Gas-phase nanoparticles and adsorbed nanoparticles structural parameters

Below are presented the structural parameters for the gas-phase nanoparticles and the adsorbed nanoparticles along with a picture for each structure.

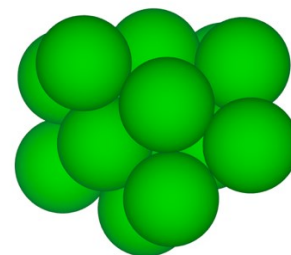
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0.0000000000000000 12.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.0000000000000000
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4
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0.6616503701653482 0.4478093842251024 0.5937805124573715
0.6566793773784056 0.4532046947345236 0.4128836518667759



Ni₉
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0.0000000000000000 14.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
Ni
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0.5412515310373134 0.5708557419018827 0.6678330509155366
0.6792948135328817 0.5401381793336286 0.4157060953085247
0.5955919853945394 0.3970773855034903 0.4656371333053460
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Ni₁₃
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0.0000000000000000 14.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
Ni
13
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Ni16

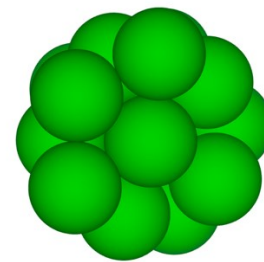
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Ni

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0.5860197624731076 0.5320506168637028 0.4367563444405491
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Ni29

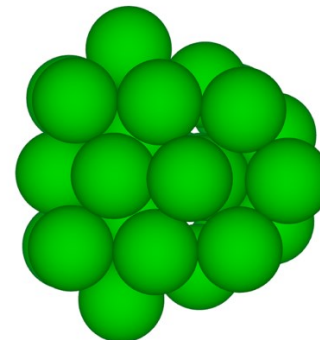
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Ni

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Ti C Ni4

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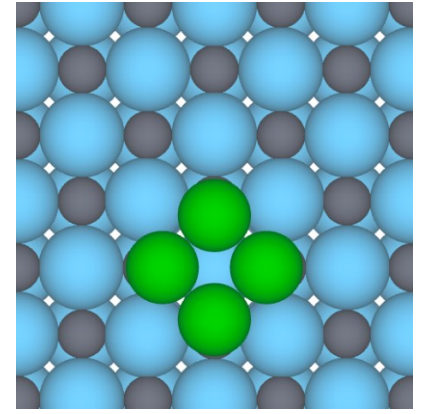
Ti C Ni

72 72 4

Selective dynamics

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0.5000000000000000	0.5000000000000000	0.0915341039999973	F	F	F
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0.6666666666666643	0.6666666666666643	0.0915341039999973	F	F	F
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Ti C Ni9

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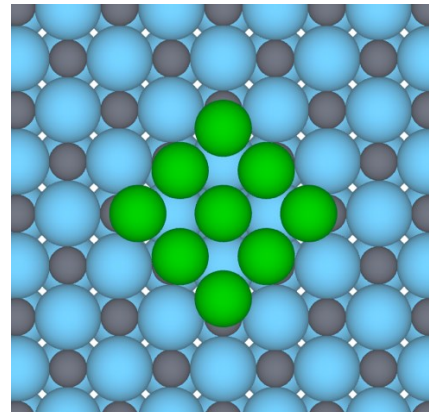
Ti C Ni

128 128 9

Selective dynamics

Direct

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Ti C Ni13

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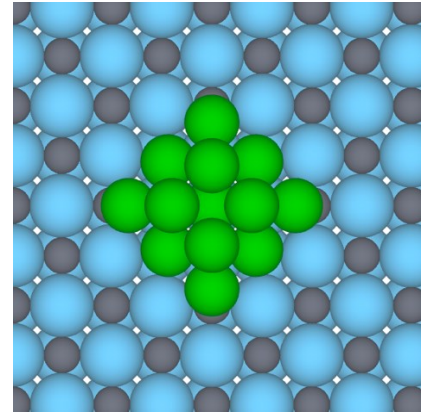
Ti C Ni

128 128 13

Selective dynamics

Direct

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0.6247615113971194	0.4999859577908129	0.2698549101528950	T	T	T
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Ti C Ni16

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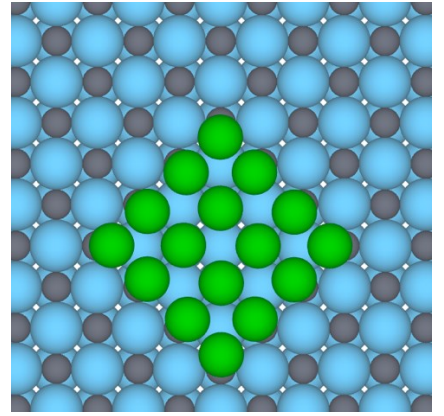
Ti C Ni

200 200 16

Selective dynamics

Direct

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Ti C Ni16

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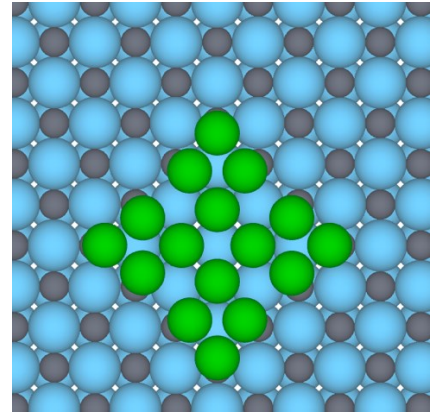
Ti C Ni

200 200 16

Selective dynamics

Direct

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Ti C Ni29

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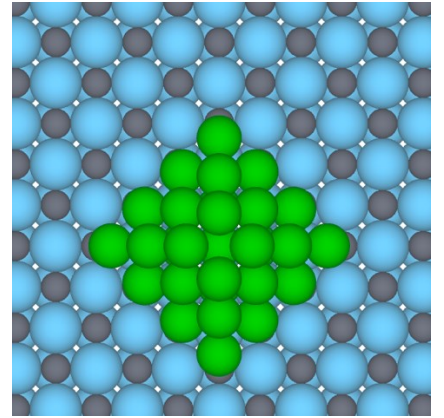
Ti C Ni

200 200 29

Selective dynamics

Direct

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