1	Electronic Supplementary Information
2	for
3	Effect of point defects on acetylene hydrogenation reaction over
4	Ni (111) surface: a density functional theory study
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1 1. The structure of Ni unit cell



2

3 Fig. S1 Ni optimized cell. (a = b = c = 3.516 Å), and $\alpha = \beta = \gamma = 90^{\circ}$.

4

8

5 2. Energy test for slab-thickness

6 Table S1 The calculated adsorption energies (E_{ad} , in eV) of C_2H_2 and C_2H_3 on the Ni

7 (111) surface with different layers

	Bottom-layer fixed (eV)		Full rela	ixed (eV)
	C ₂ H ₂ (ad)	C ₂ H ₃ (ad)	C ₂ H ₂ (ad)	C ₂ H ₃ (ad)
2-slab	-2.324	-2.134	-2.425	-2.236
3-slab	-2.556	-2.866	-2.554	-2.763
4-slab	-2.549	-2.865	-2.504	-2.694

As are shown at **Table S2** and **Fig. S2**, the adsorption energies of C_2H_4 and the energy barriers of C_2H_4 hydrogenation step ($C_2H_4*+H*\rightarrow C_2H_5*$) on the Ni(111), Ni(111) (DC=0.0500), Ni(111) (DC=0.0625) and Ni(111) (DC=0.0833) surfaces with full relaxed 3-layers slab are calculated. The errors of adsorption energies between 3 layers slab with one layer fixed and full relaxed are about 0.02 eV. The selectivity (ΔE_a) is further calculated, ΔE_a of the Ni(111)(DC=0.0625) surface with bottom layer fixed and full relaxed are 0.16 eV and 0.24 eV, respectively. The two are very similar. As shown in Table S2, the Ni(111)(DC=0.0625) surface still has the highest
 selectivity for acetylene hydrogenation, which consistent with previous model
 calculations for the fixed bottom layer. Therefore, we believe that it is relatively
 reasonable to design fixed bottom models for the study of acetylene hydrogenation
 reactions.

6

7 Table S2 The calculated adsorption energies (E_{ad} , in eV) of C_2H_4 and C_2H_5 on the

	Bottom-layer fixed (eV) C ₂ H ₄ (ad) C ₂ H ₅ (ad)		Full re	axed (eV)
			C ₂ H ₄ (ad)	C ₂ H ₅ (ad)
Ni(111)	-0.75	-1.43	-0.73	-1.40
DC=0.0500	-0.98	-2.30	-0.99	-2.32
DC=0.0625	-0.89	-2.16	-0.90	-2.12
DC=0.0833	-1.10	-2.18	-1.08	-2.17

8 models with 3-layers slab

9



11 Fig. S2 Energy profiles of the reaction $C_2H_4*+H*\rightarrow C_2H_5*$ on Ni(111), Ni(111)

- 1 (DC=0.0500), Ni(111) (DC=0.0625) and Ni(111) (DC=0.0833) surfaces (3 layers slab,
- 2 full relaxed) respectively.
- 3

	$\Delta E_{a}/\mathrm{eV}$					
	Bottom-layer fixed	Full relaxed				
Ni(111)	-0.36	-0.29				
DC=0.0500	-0.43	-0.40				
DC=0.0625	0.16	0.20				
DC=0.0833	-0.44	-0.42				

4 **Table S3** The data of ΔE_a on the models with 3-slab layer

5

6 As shown in Table S4, the difference between the adsorption energy of C_2H_2 on the 3 and 4 layers is very small, the relative errors are -0.391%, 0.385%, -0.394% 7 and 1.145%, respectively. As the defect concentration increases, the adsorption 8 strength of C2H2 first increases, then decreases, and finally increases again. The trend 9 of change is similar to that of 3-layer slab. For the 3 layers model, the intermediates 10 involved in the reaction basically tend to be adsorbed on the Ni sites near the defect (3 11 12 layers), thus the exposed sub-surface Ni sites are not involved. All models are obtained after screening. Therefore these models of 3-layer slab in our work are 13 relatively stable and reasonable, and the results obtained are also reliable. 14

16	Table S4 The calculated adsorption energies (E_{ad} , in eV) of C ₂ H ₂ on the models with
17	4 layers slabs

	Ni(111)	DC=0.0500	DC=0.0625	DC=0.0833
3-slab	-2.56	-2.60	-2.54	-2.62

4-slab	-2.55	-2.61	-2.53	-2.65
Relative error/%	-0.391	0.385	-0.394	1.145

2

3 3. The formation energy of the Ni-vacancies

In Fig. S3, the formation energies (FE) for Ni-vacancies are used in analyzing Ni 4 vacancy formation, defined as^{S1} $FE = E_{Ni-vacancies} + E_{Ni} - E_{slab}$, where $E_{Ni-vacancies}$, E_{Ni} , and 5 E_{slab} are the total energies for the Ni vacancy slab, the single Ni atom in the gas phase 6 7 (here is the energy of 1/4 Ni₄ unit cell), and the clean surface, respectively. The formation energy of the surface Ni-vacancies are 1.03 eV(DC=0.0500), 1.07 8 eV(DC=0.0625) and 1.08 eV(DC=0.0833). The fitting plot of the formation energy of 9 the surface Ni-vacancies vs defect concentration on Ni(111) surfaces are shown in Fig. 10 S4. The fits are good for these surfaces, which show that the increase in the defect 11 12 concentration results in an increase in the formation energy of the Ni-vacancies.



13

14 Fig. S3 Top views of the optimized structures of (a) pure Ni(111), (b) DC=0.0500 (c)
15 DC=0.0625 and (d) DC=0.0833 systems, along with the surface Ni vacancies
16 formation energies (*FE*) in eV. (Ni: bule).



2 Fig. S4 The fitting plot of the formation energy of the surface Ni-vacancies vs defect3 concentration on Ni(111) surfaces.

1

5 The bulk Ni vacancies formation energies (FE) are given in Fig. S5. Compared with the formation energy of surface Ni defects (DC=0.0500: FE=1.03eV; 6 DC=0.0625: FE=1.07eV; DC=0.0833: FE=1.08eV), the formation energy of bulk Ni 7 vacancies is the largest (DC=0.0500: FE=1.08eV; DC=0.0625: FE=1.12eV; 8 DC=0.0833: FE=1.13eV). It shows that bulk Ni defects are difficult to generate. As 9 the defect concentration increases, the formation energy of Ni vacancies increases. 10 11 With the same defect concentration, the formation energy of bulk defects is greater than that of surface defects. Therefore it is reasonable to study the surface defect 12 model (Fig. S6). 13



Fig. S5 Top views of the optimized structures of (a) DC=0.0500 (b) DC=0.0625 and
 (c) DC=0.0833 systems with Ni vacancies, along with the bulk Ni vacancies
 formation energies (*FE*) in eV. (Ni: bule).

4





6 Fig. S6 The formation energy (FE) of Ni vacancy as a function of defect7 concentrations.

8

9 In Fig. S7, observed in bulk as a function of defect concentration, as the 10 concentration of bulk defects increases, the interlayer distance decreases. While 11 surface defects have a great influence on the distance from the surface to the second 12 layer, and the layer spacing decreases with the increase of the defect concentration, 13 and has almost no effect on the distance between the second layer and the third layer. 14 The side proves that it is reasonable to the 3-slab model of the bottom layer fixed 15 (Table S5).



2 Fig. S7 The interlayer distances as a function of defect concentrations

	Surfac	e defect	Bulk d	lefect
	interlayer distance/Å		interlayer d	listance/Å
	1^{st} and 2^{nd} 2^{nd} and 3^{rd}		1^{st} and 2^{nd}	2^{nd} and
	layer layer		layer	3 rd layer
Ni(111)	2.000	2.010	2.000	2.010
DC=0.0500	1.998	2.011	1.992	1.996
DC=0.0625	1.994	2.010	1.987	1.994
DC=0.0833	1.989	2.010	1.985	1.990

4 Table S5. The interlayer distances of surface defect and bulk defect systems

5

6 The Ni vacancies formation energies (*FE*) of Ni₇ particle model are given in **Fig.** 7 **S8**. Compared with the formation energy of surface Ni defects, the formation energy 8 of Ni vacancies on the Ni₇ particle model is the largest (*FE* =1.25 eV). It shows that 9 surface Ni defects are easier to generate. The concentration is calculated according to 10 the formula (1), three sizes of supercells $p(4 \times 5 \times 1)$, $p(4 \times 4 \times 1)$, and $p(4 \times 3 \times 1)$ are 11 constructed to realize the change of defect concentrations. (111) surface in this work is the 12 most exposed surface of nanoparticles and the most reactive surface. Usually, the model we calculate by using the VASP software package⁴⁴⁻⁴⁶ is assumed to operate
 under 0 K conditions, rather than high temperature. Therefore, it is reasonable to
 design the surface defect model.

4



6 Fig. S8 The optimized structures of Ni₇ and Ni₇ cluster with Ni vacancy, along with

7 the Ni vacancies formation energies (FE) in eV. (Ni: bule).

8

5

⁹ 4. Surface Adsorption



Fig. S9 Adsorption structures of C₂H₂ on perfect (a) Ni (111) surface and
defective surfaces. 0.0500(b), 0.0625(c) and 0.0833(d) represent three different
defect concentrations. The numbers (in e) are the valence electrons by Bader
charge analyses. Blue: Ni atom; Dark gray: C atom; White: H atom.



- 1
- **2** Fig. S10 The optimized structures of C_2H_2 , C_2H_3 and C_2H_4 molecules (Å).
- 3

⁴ Table S6 The bond length data for C_2H_2 species in gas phase and absorbed

	<i>d</i> _{H1-C1} (Å)	<i>d</i> _{C1-C2} (Å)	<i>d</i> _{С2-H2} (Å)	d _{C1-surface}	<i>d</i> _{C2-surface}
Gas	1.070	1.208	1.070	_	_
Perfect Ni(111)	1.099	1.400	1.100	1.408	1.407
DC=0.0500	1.100	1.402	1.104	1.395	1.367
DC=0.0625	1.098	1.401	1.102	1.401	1.382
DC=0.0833	1.101	1.403	1.105	1.397	1.381

⁶ Table S7 The bond length data for C_2H_3 species in gas phase and absorbed

	<i>d</i> _{H1-C1} (Å)	<i>d</i> _{C1-C2} (Å)	<i>d</i> _{С2-H2} (Å)	<i>d</i> _{С2-H3} (Å)	d _{C1-surface}	<i>d</i> _{C2-surface}
Gas	1.072	1.291	1.106	1.106	—	_
Perfect Ni(111)	1.147	1.415	1.096	1.095	2.126	1.440
DC=0.0500	1.105	1.442	1.098	1.157	1.559	1.407
DC=0.0625	1.140	1.403	1.095	1.095	1.996	1.389
DC=0.0833	1.125	1.427	1.093	1.095	2.001	1.364

	<i>d</i> _{H1-C1} (Å)	<i>d</i> _{H2-C1} (Å)	d _{C1-C2} (Å)	d _{С2-Н3} (Å)	<i>d</i> _{C2-H4} (Å)	<i>d</i> _{C1-surface}	<i>d</i> _{C2-surface}
Gas	1.091	1.091	1.334	1.091	1.091	_	_
Ni(111)	1.094	1.094	1.442	1.114	1.119	2.123	1.756
DC=0.0500	1.095	1.093	1.425	1.095	1.122	1.701	1.664
DC=0.0625	1.092	1.136	1.453	1.094	1.118	1.891	1.714
DC=0.0833	1.094	1.122	1.455	1.097	1.128	2.012	1.679

¹ Table S8 The bond length data for C_2H_4 species in gas phase and absorbed

³ 5. van der Waals corrections

The van der Waals (vdW) interactions are described using the long range dispersion correction (DFT-D) approach. As exhibited in **Fig. S11** and **Table S9-11**, the adsorption energies of C₂H₂, C₂H₃ and C₂H₄ on Ni (111) surface and three defective Ni (111) surfaces are enhanced when considering vdW correction, and it can be seen that the vdW force only affects the energy, but not the geometry.^{S2} And the change trend of adsorption energy is consistent with the uncorrected data. Thus the structure data results in our work are relatively reasonable.



2 Fig. S11 Adsorption structures and energies with van der Waals correction of C₂H₂,
3 C₂H₃ and C₂H₄ on perfect (a) Ni (111) surface and defective surfaces. 0.0500(b),
4 0.0625(c) and 0.0833(d) represent three different defect concentrations.

5

6 Table S9 Adsorption energies (E_{ads}), adsorption energies with van der Waals
7 interaction correction (E_{vdW}) of C₂H₂

C ₂ H ₂ -ads	E _{ads} (eV)	$E_{\rm vdW}$ (eV)
Ni(111)	-2.56	-2.92
DC=0.0500	-2.60	-2.96
DC=0.0625	-2.54	-2.90
DC=0.0833	-2.62	-2.98

8

9 Table S10 Adsorption energies (E_{ads}), adsorption energies with van der Waals
10 interaction correction (E_{vdW}) of C₂H₃

C ₂ H ₃ -ads	E _{ads} (eV)	$E_{\rm vdW}$ (eV)
	S13	

2 Table S11 Adsorption energies (E_{ads}), adsorption energies with van der Waals
3 interaction correction (E_{vdW}) of C₂H₄

C ₂ H ₄ -ads	E _{ads} (eV)	$E_{\rm vdW}$ (eV)
Ni(111)	-0.75	-1.10
DC=0.0500	-0.98	-1.33
DC=0.0625	-0.89	-1.23
DC=0.0833	-1.10	-1.44

4

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⁶ 6. The data of E, $E_{entropy}$ and $E_{entropy+ZPE}$

7 The co-adsorption energy is calculated according to eqn 2: E_{ad} = E_{total} - (E_{slab}+E_g).
8 The co-adsorption energies (E_{ad}) of the C₂+H species adsorbed on all surfaces are
9 calculated from the energy difference between the optimized surface containing the
10 co-adsorbates (E_{total}) and the optimized clean surface with the C₂ molecule and H
11 atom optimized in gas state (E_{slab}+E_g).

12

13 Table S12 Total energies (*E*), total energies with entropy effect correction ($E_{entropy}$) **14** and total energies with entropy effect and zero-point energy correction ($E_{entropy+ZPE}$) of **15** the reaction intermediates

<i>E</i> (eV)	E _{entropy} (eV)	E _{entropy+ZPE} (eV)

	$H+C_{2}H_{2}\left(IS1\right)$	-218.34	-218.37	-216.71
	TS1	-217.29	-217.32	-215.70
Prefect	$H+C_{2}H_{3}$ (IS2)	-221.68	-221.71	-219.79
Ni(111)	TS2	-221.06	-221.09	-219.21
	$\mathrm{H+C_{2}H_{4}}\left(\mathrm{IS3}\right)$	-225.49	-225.53	-223.32
	TS3	-225.05	-225.09	-222.92
	$H+C_{2}H_{2}\left(IS1\right)$	-331.46	-331.56	-330.61
	TS1	-330.45	-330.52	-329.62
	$H+C_{2}H_{3}$ (IS2)	-334.61	-334.75	-333.54
DC=0.0500	TS2	-334.09	-334.23	-333.04
	$H+C_{2}H_{4}\left(IS3\right)$	-338.83	-338.97	-337.43
	TS3	-338.24	-338.41	-336.89
	$H+C_{2}H_{2}\left(IS1\right)$	-269.66	-269.76	-268.82
	TS1	-268.78	-268.88	-267.96
	H+C ₂ H ₃ (IS2)	-273.18	-273.28	-272.04
DC=0.0625	TS2	-272.88	-272.98	-271.79
	H+C ₂ H ₄ (IS3)	-277.18	-277.30	-275.78
	TS3	-276.13	-276.28	-274.87
DC=0.0833	$H+C_2H_2$ (IS1)	-207.93	-208.03	-207.09
	TS1	-206.63	-206.73	-205.82
	H+C ₂ H ₃ (IS2)	-211.41	-211.51	-210.28
	TS2	-211.02	-211.10	-209.89
	H+C ₂ H ₄ (IS3)	-215.42	-215.55	-214.01

TS3	-214.73	-214.89	-213.35

t

³ 7. Data of ΔE_a

⁴ **Table S13** The data of E_a , $E_{a,hydr}$ and $E_{a,des.}$

		$E_{\rm a,hydr}$ (eV)	$ E_{a,des} $ (eV)	$\Delta E_{\rm a}({\rm eV})$
	Perfect Ni(111)	0.39	0.75	-0.36
	DC=0.0500	0.55	0.98	-0.43
	DC=0.0625	1.05	0.89	0.16
	DC=0.0833	0.66	1.10	-0.44
5				

6



8 Fig. S12 The fitting plot of d-band center vs. energies barriers (E_a) of C₂H₄
9 hydrogenation (H*+C₂H₄*→C₂H₅*) on the perfect Ni (111) and defective (DC=0.0500,
10 DC=0.0625 and DC=0.0833) Ni(111) surfaces.

- 11
- 12

¹ 8. H₂ dissociation



Fig. S13 The structures of hydrogen before (left) and after (right) adsorption on each
defective Ni(111) surface. Blue: Ni atom, white: H atom. H₂ directly splits into two
hydrogen atoms in the adsorption process.

- 7
- ⁸ 9. Adsorption site test



2 Fig. S14 The adsorption energies for C₂ species at different sites over
3 Ni(111)(DC=0.0500) defective surface.



2 Fig. S15 The adsorption energies for C_2 species at different sites over 3 Ni(111)(DC=0.0625) defective surface.



2 Fig. S16 The adsorption energies for C₂ species at different sites over
3 Ni(111)(DC=0.0833) defective surface.

1 10. Structures of reactants, transition states and products

After the gas mixture of H₂ and C₂H₂ is injected into the reactor, H atoms come
from H₂ dissociation co-adsorbed in the vicinity of the adsorbed C₂H₂ on the surfaces
of the catalysts preparing for hydrogenation. When the reaction proceeds, the H atoms
move toward the adsorbed C₂H₂ and hydrogenate it to C₂H₄, formed via the
intermediate C₂H₃.

On the Ni (111)(DC=0.0500), C₂H₂ hydrogenation (H*+C₂H₂* \rightarrow C₂H₃*) through 7 8 a transition state with C₂H₂ at the Ni hollow site and H near the Ni top site. The 9 distance between the attacking H atom and the acceptor C atom at the transition state is 1.61 Å, which is 1.36 Å shorten than that at the initial state (Fig. S17). For 10 $H^{*+}C_{2}H_{3}^{*} \rightarrow C_{2}H_{4}^{*}$, in the initial state, $C_{2}H_{3}^{*}$ is adsorbed at the Ni hollow site, H^{*} 11 moves from Ni hollow site to Ni top site, close to the C atom of C₂H₃*. The distance 12 between C₂H₃* and H* shortens from 2.64 Å to 1.67 Å (Fig. S18). The distance 13 between the attacking H atom and the acceptor C atom decreases from 3.99 Å to 1.47 14 Å for $H^*+C_2H_4^* \rightarrow C_2H_5^*$ process(Fig. S19). 15



Reaction coordinate

17 Fig. S17 $C_2H_2*+H*\rightarrow C_2H_3*$ on Ni(111)(DC=0.0500): The hydrogen attacks the 18 acetylene (initial state before hydrogenation, IS) to form vinyl (final state after

1 hydrogenation, FS) via the transition state (TS).



3 Fig. S18 C₂H₃*+H*→C₂H₄* on Ni(111)(DC=0.0500): The hydrogen attacks the
4 acetylene (initial state before hydrogenation, IS) to form ethylene (final state after
5 hydrogenation, FS) via the transition state (TS).



6

2

7 Fig. S19 C₂H₄*+H*→C₂H₅* on Ni(111)(DC=0.0500): The hydrogen attacks the
8 acetylene (initial state before hydrogenation, IS) to form ethyl (final state after
9 hydrogenation, FS) via the transition state (TS).

10

On the Ni (111)(DC=0.0625), C₂H₂ hydrogenation (H*+C₂H₂*→C₂H₃*) through
a transition state with C₂H₂ at the Ni hollow site and H at the Ni top site. The distance
between the attacking H atom and the acceptor C atom at the transition state is 1.15 Å,
which is 1.81 Å shorten than that at the initial state (Fig. S20). For
H*+C₂H₃*→C₂H₄*, C₂H₃* is adsorbed at the Ni hollow site, H* moves from Ni

hollow site to Ni bridge site, close to the C atom of C₂H₃* at the initial state. The
 distance between C₂H₃* and H* shortens from 2.83 Å to 1.74 Å (Fig. S21). The
 distance between the attacking H atom and the acceptor C atom decreases from 3.19
 Å to 1.70 Å for H*+C₂H₄*→C₂H₅* process(Fig. S22).



6

5

7 Fig. S20 C₂H₂*+H*→C₂H₃* on Ni(111)(DC=0.0625): The hydrogen attacks the
8 acetylene (initial state before hydrogenation, IS) to form vinyl (final state after
9 hydrogenation, FS) via the transition state (TS).



11 Fig. S21 $C_2H_3^*+H^*\rightarrow C_2H_4^*$ on Ni(111)(DC=0.0625): The hydrogen attacks the 12 acetylene (initial state before hydrogenation, IS) to form ethylene (final state after

1 hydrogenation, FS) via the transition state (TS).

2



4 Fig. S22 C₂H₄*+H*→C₂H₅* on Ni(111)(DC=0.0625): The hydrogen attacks the
5 acetylene (initial state before hydrogenation, IS) to form ethyl (final state after
6 hydrogenation, FS) via the transition state (TS).

7

3

On the Ni (111)(DC=0.0833), C₂H₂ hydrogenation (H*+C₂H₂* \rightarrow C₂H₃*) through 8 9 a transition state with C₂H₂ at the Ni hollow site and H near the Ni top site. The distance between the attacking H atom and the acceptor C atom at the transition state 10 is 1.52 Å, which is 1.44 Å shorten than that at the initial state (Fig. S23). For 11 $H^{*+}C_{2}H_{3}^{*} \rightarrow C_{2}H_{4}^{*}$, in the initial state, $C_{2}H_{3}^{*}$ is adsorbed at the Ni hollow site, H^{*} 12 moves from Ni hollow site to Ni top site, close to the C atom of C₂H₃*. The distance 13 between C₂H₃* and H* shortens from 2.82 Å to 1.74 Å (Fig. S24). The distance 14 between the attacking H atom and the acceptor C atom decreases from 3.02 Å to 1.56 15 16 Å for $H^*+C_2H_4^* \rightarrow C_2H_5^*$ process(Fig. S25).



Fig. S23 $C_2H_2*+H*\rightarrow C_2H_3*$ on Ni(111)(DC=0.0833): The hydrogen attacks the 2 3 acetylene (initial state before hydrogenation, IS) to form vinyl (final state after hydrogenation, FS) via the transition state (TS). 4 5

0.4 TS(0.38) 0.3 Energy(eV) 0.0 0.0 -0.1 -0.2 **Reaction coordinate**

1



Fig. S24 $C_2H_3^*+H^*\rightarrow C_2H_4^*$ on Ni(111)(DC=0.0833): The hydrogen attacks the 7 8 acetylene (initial state before hydrogenation, IS) to form ethylene (final state after 9 hydrogenation, FS) via the transition state (TS).



2 Fig. S25 C₂H₄*+H*→C₂H₅* on Ni(111)(DC=0.0833): The hydrogen attacks the
3 acetylene (initial state before hydrogenation, IS) to form ethyl (final state after
4 hydrogenation, FS) via the transition state (TS).

1

6 Table S14 Summary of ΔE_a (in eV) of Reported Literatures

Catalyst	Selectivity(ΔE_{a} , eV)	Reference
Pd(111)	0.06	
Pd(100)	-0.30	J Catal. 2013.305, 264
Pd(211)	-0.45	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Pd(211)-defect	-0.38	
Cu ₁₃	-0.32	I Phys Chem C 2019 123
Cu ₅₅	-0.24	16107–16117
Pd ₁₃	-0.24	10107 10117
Ni(111)	0.12	
Au-Ni(111)	0.33	ACS Catal., 2012, 2, 1027
Ag-Ni(111)	0.41	

Cu-Ni(111)	0.11	
Ni ₃ Sn(111)	0.37	
Ni ₃ Sn(001)	0.56	
Ni ₃ Sn ₂ (101)	0.48	Phys. Chem. Chem. Phys., 2019,
Ni ₃ Sn ₂ (001)	0.14	21, 1384
Ni ₃ Sn ₂ (101)-2	-0.15	
Ni ₃ Sn ₂ (001)-2	-0.21	
NiGa(110)	0.25	Dalton Trans., 2018, 47, 4198
Ni3Ga (111)	0.28	Cham Sai 2010 10 (14
Ni (111)	-0.36	<i>Chem. Sci.</i> , 2019, 10, 014
PdZn-1.2@ZIF-8C	0.27	
PdZn-10/ZIF-8C	-0.11	Aav. Mater., 2018, 30, 1801878

2

3 Reference

- 4 (S1) Ind. Eng. Chem. Res. 2018, 57, 6830–6841.
- 5 (S2) Appl. Surf. Sci., 2018, 435, 521–528.