

# Francesc Vies

## List of Publications by Citations

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147  
papers

5,667  
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40  
h-index

70  
g-index

159  
ext. papers

6,577  
ext. citations

6.8  
avg, IF

6.26  
L-index

#	Paper	IF	Citations
147	Competition for graphene: graphynes with direction-dependent Dirac cones. <i>Physical Review Letters</i> , <b>2012</b> , 108, 086804	7.4	809
146	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 3832-9	6.4	187
145	A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 174709	3.9	157
144	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 1631-40	6.4	153
143	Atomic and electronic structure of molybdenum carbide phases: bulk and low Miller-index surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 12617-25	3.6	151
142	Graphene on Ni(111): Coexistence of Different Surface Structures. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 759-764	6.4	139
141	Understanding the reactivity of metallic nanoparticles: beyond the extended surface model for catalysis. <i>Chemical Society Reviews</i> , <b>2014</b> , 43, 4922-39	58.5	132
140	The bending machine: CO <sub>2</sub> activation and hydrogenation on $\epsilon$ -MoC(001) and $\epsilon$ -Mo <sub>2</sub> C(001) surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 14912-21	3.6	131
139	Bonding Mechanisms of Graphene on Metal Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 7360-7368	10.4	121
138	Transition metal carbides as novel materials for CO <sub>2</sub> capture, storage, and activation. <i>Energy and Environmental Science</i> , <b>2016</b> , 9, 141-144	35.4	115
137	Methane activation by platinum: critical role of edge and corner sites of metal nanoparticles. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 6530-9	4.8	112
136	Transition metal adatoms on graphene: A systematic density functional study. <i>Carbon</i> , <b>2015</b> , 95, 525-534	10.4	103
135	CO <sub>2</sub> abatement using two-dimensional MXene carbides. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 3381-3385	33.85	93
134	Highly Active Au/ $\epsilon$ -MoC and Cu/ $\epsilon$ -MoC Catalysts for the Conversion of CO <sub>2</sub> : The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 8269-78	16.4	92
133	Bandgap engineering of graphene by physisorbed adsorbates. <i>Advanced Materials</i> , <b>2011</b> , 23, 2638-43	24	75
132	The conversion of CO <sub>2</sub> to methanol on orthorhombic $\epsilon$ -Mo <sub>2</sub> C and Cu/ $\epsilon$ -Mo <sub>2</sub> C catalysts: mechanism for admetal induced change in the selectivity and activity. <i>Catalysis Science and Technology</i> , <b>2016</b> , 6, 6766-6777	5.5	74
131	Growth and electronic structure of nitrogen-doped graphene on Ni(111). <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	73

130	Effective and Highly Selective CO Generation from CO <sub>2</sub> Using a Polycrystalline $\beta$ -Mo <sub>2</sub> C Catalyst. <i>ACS Catalysis</i> , <b>2017</b> , 7, 4323-4335	13.1	68
129	Catalyst size matters: Tuning the molecular mechanism of the water-gas shift reaction on titanium carbide based compounds. <i>Journal of Catalysis</i> , <b>2008</b> , 260, 103-112	7.3	67
128	Edge sites as a gate for subsurface carbon in palladium nanoparticles. <i>Journal of Catalysis</i> , <b>2009</b> , 266, 59-63	7.3	64
127	Desulfurization of thiophene on Au/TiC(001): Au-C interactions and charge polarization. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 8595-602	16.4	64
126	Dissociation of SO <sub>2</sub> on Au/TiC(001): effects of Au-C interactions and charge polarization. <i>Angewandte Chemie - International Edition</i> , <b>2008</b> , 47, 6685-9	16.4	64
125	On the interaction of polycyclic aromatic compounds with graphene. <i>Carbon</i> , <b>2012</b> , 50, 2482-2492	10.4	61
124	Density Functional Study of the Adsorption of Atomic Oxygen on the (001) Surface of Early Transition-Metal Carbides. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 1307-1314	3.8	61
123	Adsorption of gold on TiC(001): Au-C interactions and charge polarization. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 211102	3.9	59
122	A Systematic Density Functional Study of Molecular Oxygen Adsorption and Dissociation on the (001) Surface of Group IV-VI Transition Metal Carbides. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 16982-16989	3.8	58
121	Brdsted-Evans-Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 4168-4171	3.8	56
120	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. <i>Theoretical Chemistry Accounts</i> , <b>2008</b> , 120, 565-573	1.9	56
119	Functionalization of $\beta$ -graphyne by transition metal adatoms. <i>Carbon</i> , <b>2017</b> , 120, 63-70	10.4	55
118	Formation of one-dimensional electronic states along the step edges of CeO <sub>2</sub> (111). <i>ACS Nano</i> , <b>2012</b> , 6, 1126-33	16.7	55
117	Charge polarization at a Au-TiC interface and the generation of highly active and selective catalysts for the low-temperature water-gas shift reaction. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 11270-4	16.4	54
116	Theoretical assessment of graphene-metal contacts. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 244701	3.9	53
115	SO <sub>2</sub> Adsorption on Pt(111) and Oxygen Precovered Pt(111): A Combined Infrared Reflection Absorption Spectroscopy and Density Functional Study. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 479-491	3.8	53
114	Fundamentals of Methanol Synthesis on Metal Carbide Based Catalysts: Activation of CO <sub>2</sub> and H <sub>2</sub> . <i>Topics in Catalysis</i> , <b>2015</b> , 58, 159-173	2.3	50
113	MXenes as promising catalysts for water dissociation. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 260, 118118	11.8	49

112	On the mechanism of formation of metal nanowires by self-assembly. <i>Angewandte Chemie - International Edition</i> , <b>2007</b> , 46, 7094-7	16.4	48
111	Systematic study of the effect of HSE functional internal parameters on the electronic structure and band gap of a representative set of metal oxides. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 7813-789	3.5	47
110	Jacob's Ladder as Sketched by Escher: Assessing the Performance of Broadly Used Density Functionals on Transition Metal Surface Properties. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 395-403	6.4	44
109	Size dependent structural and polymorphic transitions in ZnO: from nanocluster to bulk. <i>Nanoscale</i> , <b>2017</b> , 9, 10067-10074	7.7	42
108	Carbon on platinum substrates: from carbidic to graphitic phases on the (111) surface and on nanoparticles. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 11963-73	2.8	41
107	Density functional calculations of Pd nanoparticles using a plane-wave method. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 8911-5	2.8	40
106	Interaction of oxygen with ZrC(001) and VC(001): Photoemission and first-principles studies. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	40
105	Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials. <i>Nature Communications</i> , <b>2017</b> , 8, 1957	17.4	38
104	A Combined Density-Functional and IRAS Study on the Interaction of NO with Pd Nanoparticles: Identifying New Adsorption Sites with Novel Properties. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 16539-16549	3.8	38
103	Assessing GW Approaches for Predicting Core Level Binding Energies. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 877-883	6.4	37
102	Unravelling Morphological and Topological Energy Contributions of Metal Nanoparticles.. <i>Nanomaterials</i> , <b>2021</b> , 12,	5.4	37
101	On the prediction of core level binding energies in molecules, surfaces and solids. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 8403-8410	3.6	35
100	Absolute Surface Step Energies: Accurate Theoretical Methods Applied to Ceria Nanoislands. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 1956-1961	6.4	35
99	Novel Au <sub>3</sub> TiC catalysts for CO oxidation and desulfurization processes. <i>Catalysis Today</i> , <b>2011</b> , 166, 2-9	5.3	35
98	Predicting core level binding energies shifts: Suitability of the projector augmented wave approach as implemented in VASP. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 518-522	3.5	34
97	Adsorption and dissociation of molecular hydrogen on orthorhombic EMo <sub>2</sub> C and cubic EMoC (001) surfaces. <i>Surface Science</i> , <b>2017</b> , 656, 24-32	1.8	34
96	Room Temperature Methane Capture and Activation by Ni Clusters Supported on TiC(001): Effects of Metal-Carbide Interactions on the Cleavage of the C-H Bond. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 5303-5313	16.4	33
95	Hydroxyl Identification on ZnO by Infrared Spectroscopies: Theory and Experiments. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 1492-1505	3.8	33

94	Influence of the surface dipole layer and Pauli repulsion on band energies and doping in graphene adsorbed on metal surfaces. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	33
93	Two-dimensional nitrides as highly efficient potential candidates for CO capture and activation. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 17117-17124	3.6	33
92	Performance of the TPSS Functional on Predicting Core Level Binding Energies of Main Group Elements Containing Molecules: A Good Choice for Molecules Adsorbed on Metal Surfaces. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 324-31	6.4	32
91	Adding Pieces to the CO/Pt(111) Puzzle: The Role of Dispersion. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 3970-3977	3.8	31
90	Morphology effects in photoactive ZnO nanostructures: photooxidative activity of polar surfaces. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 8782-8792	13	31
89	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. <i>ACS Catalysis</i> , <b>2020</b> , 10, 5049-5056	13.1	31
88	Thickness biased capture of CO on carbide MXenes. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 23136-23142	3.2	31
87	Critical effect of carbon vacancies on the reverse water gas shift reaction over vanadium carbide catalysts. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 267, 118719	21.8	30
86	Role of kinetics in the selective surface oxidations of transition metal carbides. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 15454-8	3.4	29
85	Matildite versus schapbachite: First-principles investigation of the origin of photoactivity in AgBiS <sub>2</sub> . <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	29
84	Highly active Au/EMoC and Au/EMo <sub>2</sub> C catalysts for the low-temperature water gas shift reaction: effects of the carbide metal/carbon ratio on the catalyst performance. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 5332-5342	5.5	26
83	Tuning the surface chemistry of Pd by atomic C and H: a microscopic picture. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 1335-45	4.8	26
82	On the hydrogen adsorption and dissociation on Cu surfaces and nanorows. <i>Surface Science</i> , <b>2016</b> , 646, 221-229	1.8	25
81	Desulfurization Reactions on Surfaces of Metal Carbides: Photoemission and Density Functional Studies. <i>Topics in Catalysis</i> , <b>2010</b> , 53, 393-402	2.3	24
80	Effect of the Support on the Electronic Structure of Au Nanoparticles Supported on Transition Metal Carbides: Choice of the Best Substrate for Au Activation. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 19994-20001	3.8	23
79	Structure and electronic properties of Cu nanoclusters supported on Mo <sub>2</sub> C(001) and MoC(001) surfaces. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 114704	3.9	22
78	Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-Doped Graphene. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 11319-11327	3.8	21
77	Hydrogen storage on metal oxide model clusters using density-functional methods and reliable van der Waals corrections. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 5382-92	3.6	21

76	A DF-vdW study of the CH <sub>4</sub> adsorption on different Ni surfaces. <i>Surface Science</i> , <b>2014</b> , 625, 64-68	1.8	21
75	Subsurface Carbon: A General Feature of Noble Metals. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 1744-1748	16.4	20
74	Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 264, 118476	21.8	19
73	Density Functional Calculations and IR Reflection Absorption Spectroscopy on the Interaction of SO <sub>2</sub> with Oxide-Supported Pd Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 13813-13824	3.8	18
72	Kinetics of the sulfur oxidation on palladium: a combined in situ x-ray photoelectron spectroscopy and density-functional study. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 094702	3.9	18
71	Electronic-structure-based material descriptors: (in)dependence on self-interaction and Hartree-Fock exchange. <i>Chemical Communications</i> , <b>2015</b> , 51, 5602-5	5.8	17
70	Adsorption and reaction of SO <sub>2</sub> on clean and oxygen precovered Pd(100)--a combined HR-XPS and DF study. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 16227-35	3.6	17
69	Dissociation of SO <sub>2</sub> on Au/TiC(001): Effects of Au-C Interactions and Charge Polarization. <i>Angewandte Chemie</i> , <b>2008</b> , 120, 6787-6791	3.6	17
68	The interaction of CO <sub>2</sub> with sodium-promoted W(011). <i>Physical Chemistry Chemical Physics</i> , <b>2005</b> , 7, 3866-73	3.3	17
67	First-Principles Calculations on the Adsorption Behavior of Amino Acids on a Titanium Carbide MXene.. <i>ACS Applied Bio Materials</i> , <b>2020</b> , 3, 5913-5921	4.1	17
66	Elucidating the Structure of Ethanol-Producing Active Sites at Oxide-Derived Cu Electrocatalysts. <i>ACS Catalysis</i> , <b>2020</b> , 10, 10488-10494	13.1	17
65	Bandgap engineering by cationic disorder: case study on AgBiS. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 27940-27944	3.6	16
64	Performance of Minnesota functionals on predicting core-level binding energies of molecules containing main-group elements. <i>Theoretical Chemistry Accounts</i> , <b>2016</b> , 135, 1	1.9	16
63	Assessing the usefulness of transition metal carbides for hydrogenation reactions. <i>Chemical Communications</i> , <b>2019</b> , 55, 12797-12800	5.8	16
62	Cohesion and coordination effects on transition metal surface energies. <i>Surface Science</i> , <b>2017</b> , 664, 45-49.8	4.8	15
61	Biogas Upgrading by Transition Metal Carbides. <i>ACS Applied Energy Materials</i> , <b>2018</b> , 1, 43-47	6.1	15
60	Microscopic origin of n-type behavior in Si-doped AlN. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	15
59	Adsorption and diffusion of Au atoms on the (001) surface of Ti, Zr, Hf, V, Nb, Ta, and Mo carbides. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 244706	3.9	15

58	Effect of the Exchange-Correlation Potential on the Transferability of Brūsted-Evans-Polanyi Relationships in Heterogeneous Catalysis. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 2121-6 <sup>6.4</sup>	15
57	Ultra-high selectivity biogas upgrading through porous MXenes. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 12296-12300	13 14
56	On the H interactions with transition metal adatoms supported on graphene: a systematic density functional study. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 3819-3830	3.6 14
55	The contact of graphene with Ni(111) surface: description by modern dispersive forces approaches. <i>Theoretical Chemistry Accounts</i> , <b>2016</b> , 135, 1	1.9 14
54	Methane capture at room temperature: adsorption on cubic $\epsilon$ MoC and orthorhombic $\epsilon$ Mo <sub>2</sub> C molybdenum carbide (001) surfaces. <i>RSC Advances</i> , <b>2015</b> , 5, 33737-33746	3.7 14
53	MXenes atomic layer stacking phase transitions and their chemical activity consequences. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2 14
52	Combining Theory and Experiment for Multitechnique Characterization of Activated CO <sub>2</sub> on Transition Metal Carbide (001) Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 7567-7576	3.8 14
51	Electronic structure of stoichiometric and reduced ZnO from periodic relativistic all electron hybrid density functional calculations using numeric atom-centered orbitals. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 523-529	3.5 13
50	Artificial-intelligence-driven discovery of catalyst genes with application to CO activation on semiconductor oxides.. <i>Nature Communications</i> , <b>2022</b> , 13, 419	17.4 13
49	Selectivity for CO <sub>2</sub> over CH <sub>4</sub> on a functionalized periodic mesoporous phenylene-silica explained by transition state theory. <i>Chemical Physics Letters</i> , <b>2017</b> , 671, 161-164	2.5 12
48	Critical Hydrogen Coverage Effect on the Hydrogenation of Ethylene Catalyzed by $\epsilon$ MoC(001): An Ab Initio Thermodynamic and Kinetic Study. <i>ACS Catalysis</i> , <b>2020</b> , 10, 6213-6222	13.1 12
47	Mechanisms of carbon dioxide reduction on strontium titanate perovskites. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 9392-9398	13 12
46	Diversity of Adsorbed Hydrogen on the TiC(001) Surface at High Coverages. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 28013-28020	3.8 12
45	Nanoscale thermal stabilization via permutational premelting. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3 11
44	Concepts, models, and methods in computational heterogeneous catalysis illustrated through CO <sub>2</sub> conversion. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2021</b> , 11, e1530	7.9 11
43	Carbon dissolution and segregation in platinum. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 807-816	5.5 10
42	ZnO powders as multi-facet single crystals. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 10622-10628	3.6 10
41	Substrate-mediated single-atom isolation: dispersion of Ni and La on $\epsilon$ graphyne. <i>Theoretical Chemistry Accounts</i> , <b>2017</b> , 136, 1	1.9 9



40	Template-assisted formation of fullerenes from short-chain hydrocarbons by supported platinum nanoparticles. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 4611-4	16.4	9
39	Boosting the activity of transition metal carbides towards methane activation by nanostructuring. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 7110-7118	3.6	8
38	Robustness of surface activity electronic structure-based descriptors of transition metals. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 20548-20554	3.6	8
37	Tuning transition metal carbide activity by surface metal alloying: a case study on CO capture and activation. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 22179-22186	3.6	8
36	Grazynes: Carbon-Based Two-Dimensional Composites with Anisotropic Properties. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 27140-27149	3.8	8
35	Charge Polarization at a Au <sub>3</sub> SiC Interface and the Generation of Highly Active and Selective Catalysts for the Low-Temperature Water-Gas Shift Reaction. <i>Angewandte Chemie</i> , <b>2014</b> , 126, 11452-11456	3.6	8
34	Exfoliation Energy as a Descriptor of MXenes Synthesizability and Surface Chemical Activity. <i>Nanomaterials</i> , <b>2021</b> , 11,	5.4	8
33	Carbon Capture and Usage by MXenes. <i>ACS Catalysis</i> , <b>2021</b> , 11, 11248-11255	13.1	8
32	Matildite Contact with Media: First-Principles Study of AgBiS Surfaces and Nanoparticle Morphology. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 521-526	3.4	7
31	Generalized gradient approximation adjusted to transition metals properties: Key roles of exchange and local spin density. <i>Journal of Computational Chemistry</i> , <b>2020</b> , 41, 2598-2603	3.5	7
30	Optical Properties and Chemical Ordering of AgPt Nanoalloys: A Computational Study. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 25482-25491	3.8	6
29	Surface Activity of Early Transition-Metal Oxycarbides: CO <sub>2</sub> Adsorption Case Study. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 3664-3671	3.8	6
28	Towards understanding the role of carbon atoms on transition metal surfaces: Implications for catalysis. <i>Applied Surface Science</i> , <b>2020</b> , 513, 145765	6.7	6
27	On the Mechanism of Formation of Metal Nanowires by Self-Assembly. <i>Angewandte Chemie</i> , <b>2007</b> , 119, 7224-7227	3.6	6
26	Predicting the Effect of Dopants on CO <sub>2</sub> Adsorption in Transition Metal Carbides: Case Study on TiC (001). <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 15969-15976	3.8	5
25	Vacancy patterning and patterning vacancies: controlled self-assembly of fullerenes on metal surfaces. <i>Nanoscale</i> , <b>2014</b> , 6, 10850-8	7.7	5
24	When reconstruction comes around: Ni, Cu, and Au adatoms on EMoC(001). <i>Surface Science</i> , <b>2014</b> , 624, 32-36	1.8	5
23	The Ti <sub>2</sub> CO <sub>2</sub> MXene as a nucleobase 2D sensor: A first-principles study. <i>Applied Surface Science</i> , <b>2021</b> , 544, 148946	6.7	5



22	Subsurface Carbon: A General Feature of Noble Metals. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 1758-1762	3.6	5
21	Approaching the Quantitative Description of Enantioselective Adsorption by the Density Functional Theory Means. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 11714-11722	3.8	4
20	Thermodynamics and Kinetics of Molecular Hydrogen Adsorption and Dissociation on MXenes: Relevance to Heterogeneously Catalyzed Hydrogenation Reactions. <i>ACS Catalysis</i> , 12850-12857	13.1	4
19	Bulk (in)stability as a possible source of surface reconstruction. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 19249-19253	3.6	4
18	Double-well potential energy surface in the interaction between h-BN and Ni(111). <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 10888-10894	3.6	3
17	Understanding W Doping in Wurtzite ZnO. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 19082-19089	3.8	3
16	Implicit solvent effects in the determination of Brüsted-Evans-Polanyi relationships for heterogeneously catalyzed reactions. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 17687-17695	3.6	3
15	Supported Molybdenum Carbide Nanoparticles as Hot Hydrogen Reservoirs for Catalytic Applications. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 8437-8441	6.4	3
14	The nano gold rush: Graphynes as atomic sieves for coinage and Pt-group transition metals. <i>Applied Surface Science</i> , <b>2020</b> , 499, 143927	6.7	3
13	Adsorption and Activation of CO on Nitride MXenes: Composition, Temperature, and Pressure effects. <i>ChemPhysChem</i> , <b>2021</b> , 22, 2456-2463	3.2	3
12	Role of C and P Sites on the Chemical Activity of Metal Carbides and Phosphides: From Clusters to Single-Crystal Surfaces <b>2010</b> , 117-132		3
11	Explaining Cu@Pt Bimetallic Nanoparticles Activity Based on NO Adsorption. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 11478-11491	4.8	2
10	Ionic Liquid Chiral Resolution: Methyl 2-Ammonium Chloride Propanoate on Al(854)S Surface. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 1568-1575	3.8	2
9	Identifying the Atomic Layer Stacking of MoC MXene by Probe Molecule Adsorption.. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 26808-26813	3.8	2
8	Supported Molybdenum Carbide Nanoparticles as an Excellent Catalyst for CO <sub>2</sub> Hydrogenation. <i>ACS Catalysis</i> , <b>2021</b> , 11, 9679-9687	13.1	2
7	Insights on alkylidene formation on Mo <sub>2</sub> C: A potential overlap between direct deoxygenation and olefin metathesis. <i>Journal of Catalysis</i> , <b>2021</b> , 393, 381-389	7.3	1
6	Mo single atoms in the Cu(111) surface as improved catalytic active centers for deoxygenation reactions. <i>Catalysis Science and Technology</i> , <b>2021</b> , 11, 4969-4978	5.5	1
5	Size and Stoichiometry Effects on the Reactivity of MoC <sub>y</sub> Nanoparticles toward Ethylene. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 6287-6297	3.8	1

4	Simulating heterogeneous catalysis on metallic nanoparticles: From under-coordinated sites to extended facets. <i>Frontiers of Nanoscience</i> , <b>2018</b> , 101-128	0.7	1
3	Catalytic Reduction of Carbon Dioxide on the (001), (011), and (111) Surfaces of TiC and ZrC: A Computational Study.. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 5138-5150	3.8	1
2	Acetylene-Mediated Electron Transport in Nanostructured Graphene and Hexagonal Boron Nitride. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 11220-11227	6.4	0
1	Template-Assisted Formation of Fullerenes from Short-Chain Hydrocarbons by Supported Platinum Nanoparticles. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 4707-4710	3.6	