Francesc Vies

List of Publications by Year in Descending Order

147 papers	5,667 citations	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	Artificial-intelligence-driven discovery of catalyst genes with application to CO activation on semiconductor oxides.. *Nature Communications*, **2022**, 13, 419	17.4	13
146	Catalytic Reduction of Carbon Dioxide on the (001), (011), and (111) Surfaces of TiC and ZrC: A Computational Study.. *Journal of Physical Chemistry C*, **2022**, 126, 5138-5150	3.8	1
145	Identifying the Atomic Layer Stacking of MoC MXene by Probe Molecule Adsorption.. *Journal of Physical Chemistry C*, **2021**, 125, 26808-26813	3.8	2
144	Acetylene-Mediated Electron Transport in Nanostructured Graphene and Hexagonal Boron Nitride. *Journal of Physical Chemistry Letters*, **2021**, 12, 11220-11227	6.4	0
143	The Ti2CO2 MXene as a nucleobase 2D sensor: A first-principles study. *Applied Surface Science*, **2021**, 544, 148946	6.7	5
142	Concepts, models, and methods in computational heterogeneous catalysis illustrated through CO2 conversion. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1530	7.9	11
141	Insights on alkylidene formation on Mo2C: A potential overlap between direct deoxygenation and olefin metathesis. *Journal of Catalysis*, **2021**, 393, 381-389	7.3	1
140	Exfoliation Energy as a Descriptor of MXenes Synthesizability and Surface Chemical Activity. *Nanomaterials*, **2021**, 11,	5.4	8
139	Mo single atoms in the Cu(111) surface as improved catalytic active centers for deoxygenation reactions. *Catalysis Science and Technology*, **2021**, 11, 4969-4978	5.5	1
138	Size and Stoichiometry Effects on the Reactivity of MoCy Nanoparticles toward Ethylene. *Journal of Physical Chemistry C*, **2021**, 125, 6287-6297	3.8	1
137	Supported Molybdenum Carbide Nanoparticles as an Excellent Catalyst for CO2 Hydrogenation. *ACS Catalysis*, **2021**, 11, 9679-9687	13.1	2
136	Carbon Capture and Usage by MXenes. *ACS Catalysis*, **2021**, 11, 11248-11255	13.1	8
135	Adsorption and Activation of CO on Nitride MXenes: Composition, Temperature, and Pressure effects. *ChemPhysChem*, **2021**, 22, 2456-2463	3.2	3
134	Unravelling Morphological and Topological Energy Contributions of Metal Nanoparticles.. *Nanomaterials*, **2021**, 12,	5.4	37
133	Critical Hydrogen Coverage Effect on the Hydrogenation of Ethylene Catalyzed by □MoC(001): An Ab Initio Thermodynamic and Kinetic Study. *ACS Catalysis*, **2020**, 10, 6213-6222	13.1	12
132	Ultra-high selectivity biogas upgrading through porous MXenes. *Journal of Materials Chemistry A*, **2020**, 8, 12296-12300	13	14
131	Boosting the activity of transition metal carbides towards methane activation by nanostructuring. *Physical Chemistry Chemical Physics*, **2020**, 22, 7110-7118	3.6	8

130	Predicting the Effect of Dopants on CO2 Adsorption in Transition Metal Carbides: Case Study on TiC (001). *Journal of Physical Chemistry C*, **2020**, 124, 15969-15976	3.8	5
129	Explaining Cu@Pt Bimetallic Nanoparticles Activity Based on NO Adsorption. *Chemistry - A European Journal*, **2020**, 26, 11478-11491	4.8	2
128	Towards understanding the role of carbon atoms on transition metal surfaces: Implications for catalysis. *Applied Surface Science*, **2020**, 513, 145765	6.7	6
127	Critical effect of carbon vacancies on the reverse water gas shift reaction over vanadium carbide catalysts. *Applied Catalysis B: Environmental*, **2020**, 267, 118719	21.8	30
126	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. *ACS Catalysis*, **2020**, 10, 5049-5056	13.1	31
125	MXenes atomic layer stacking phase transitions and their chemical activity consequences. *Physical Review Materials*, **2020**, 4,	3.2	14
124	Supported Molybdenum Carbide Nanoparticles as Hot Hydrogen Reservoirs for Catalytic Applications. *Journal of Physical Chemistry Letters*, **2020**, 11, 8437-8441	6.4	3
123	Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. *Applied Catalysis B: Environmental*, **2020**, 264, 118476	21.8	19
122	First-Principles Calculations on the Adsorption Behavior of Amino Acids on a Titanium Carbide MXene.. *ACS Applied Bio Materials*, **2020**, 3, 5913-5921	4.1	17
121	Bulk (in)stability as a possible source of surface reconstruction. *Physical Chemistry Chemical Physics*, **2020**, 22, 19249-19253	3.6	4
120	Generalized gradient approximation adjusted to transition metals properties: Key roles of exchange and local spin density. *Journal of Computational Chemistry*, **2020**, 41, 2598-2603	3.5	7
119	Elucidating the Structure of Ethanol-Producing Active Sites at Oxide-Derived Cu Electrocatalysts. *ACS Catalysis*, **2020**, 10, 10488-10494	13.1	17
118	The nano gold rush: Graphynes as atomic sieves for coinage and Pt-group transition metals. *Applied Surface Science*, **2020**, 499, 143927	6.7	3
117	MXenes as promising catalysts for water dissociation. *Applied Catalysis B: Environmental*, **2020**, 260, 118191	21.8	49
116	Mechanisms of carbon dioxide reduction on strontium titanate perovskites. *Journal of Materials Chemistry A*, **2020**, 8, 9392-9398	13	12
115	Optical Properties and Chemical Ordering of AgPt Nanoalloys: A Computational Study. *Journal of Physical Chemistry C*, **2019**, 123, 25482-25491	3.8	6
114	Surface Activity of Early Transition-Metal Oxycarbides: CO2 Adsorption Case Study. *Journal of Physical Chemistry C*, **2019**, 123, 3664-3671	3.8	6
113	Approaching the Quantitative Description of Enantioselective Adsorption by the Density Functional Theory Means. *Journal of Physical Chemistry C*, **2019**, 123, 11714-11722	3.8	4

112	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. *Journal of the American Chemical Society*, **2019**, 141, 5303-5313	16.4	33
111	Double-well potential energy surface in the interaction between h-BN and Ni(111). *Physical Chemistry Chemical Physics*, **2019**, 21, 10888-10894	3.6	3
110	Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-Doped Graphene. *Journal of Physical Chemistry C*, **2019**, 123, 11319-11327	3.8	21
109	Implicit solvent effects in the determination of Brønsted-Evans-Polanyi relationships for heterogeneously catalyzed reactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 17687-17695	3.6	3
108	Grazynes: Carbon-Based Two-Dimensional Composites with Anisotropic Properties. *Journal of Physical Chemistry C*, **2019**, 123, 27140-27149	3.8	8
107	Assessing the usefulness of transition metal carbides for hydrogenation reactions. *Chemical Communications*, **2019**, 55, 12797-12800	5.8	16
106	Thickness biased capture of CO on carbide MXenes. *Physical Chemistry Chemical Physics*, **2019**, 21, 23136-23142	3.6	31
105	Subsurface Carbon: A General Feature of Noble Metals. *Angewandte Chemie - International Edition*, **2019**, 58, 1744-1748	16.4	20
104	Subsurface Carbon: A General Feature of Noble Metals. *Angewandte Chemie*, **2019**, 131, 1758-1762	3.6	5
103	Combining Theory and Experiment for Multitechnique Characterization of Activated CO2 on Transition Metal Carbide (001) Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 7567-7576	3.8	14
102	CO2 abatement using two-dimensional MXene carbides. *Journal of Materials Chemistry A*, **2018**, 6, 3381-3385	3.6	93
101	Biogas Upgrading by Transition Metal Carbides. *ACS Applied Energy Materials*, **2018**, 1, 43-47	6.1	15
100	Assessing GW Approaches for Predicting Core Level Binding Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 877-883	6.4	37
99	On the H interactions with transition metal adatoms supported on graphene: a systematic density functional study. *Physical Chemistry Chemical Physics*, **2018**, 20, 3819-3830	3.6	14
98	On the prediction of core level binding energies in molecules, surfaces and solids. *Physical Chemistry Chemical Physics*, **2018**, 20, 8403-8410	3.6	35
97	Matildite Contact with Media: First-Principles Study of AgBiS Surfaces and Nanoparticle Morphology. *Journal of Physical Chemistry B*, **2018**, 122, 521-526	3.4	7
96	Understanding W Doping in Wurtzite ZnO. *Journal of Physical Chemistry C*, **2018**, 122, 19082-19089	3.8	3
95	Robustness of surface activity electronic structure-based descriptors of transition metals. *Physical Chemistry Chemical Physics*, **2018**, 20, 20548-20554	3.6	8

94	Tuning transition metal carbide activity by surface metal alloying: a case study on CO capture and activation. *Physical Chemistry Chemical Physics*, **2018**, 20, 22179-22186	3.6	8
93	Jacob's Ladder as Sketched by Escher: Assessing the Performance of Broadly Used Density Functionals on Transition Metal Surface Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 395-403	6.4	44
92	Diversity of Adsorbed Hydrogen on the TiC(001) Surface at High Coverages. *Journal of Physical Chemistry C*, **2018**, 122, 28013-28020	3.8	12
91	Simulating heterogeneous catalysis on metallic nanoparticles: From under-coordinated sites to extended facets. *Frontiers of Nanoscience*, **2018**, 101-128	0.7	1
90	Two-dimensional nitrides as highly efficient potential candidates for CO capture and activation. *Physical Chemistry Chemical Physics*, **2018**, 20, 17117-17124	3.6	33
89	Carbon dissolution and segregation in platinum. *Catalysis Science and Technology*, **2017**, 7, 807-816	5.5	10
88	Adding Pieces to the CO/Pt(111) Puzzle: The Role of Dispersion. *Journal of Physical Chemistry C*, **2017**, 121, 3970-3977	3.8	31
87	Electronic structure of stoichiometric and reduced ZnO from periodic relativistic all electron hybrid density functional calculations using numeric atom-centered orbitals. *Journal of Computational Chemistry*, **2017**, 38, 523-529	3.5	13
86	Systematic study of the effect of HSE functional internal parameters on the electronic structure and band gap of a representative set of metal oxides. *Journal of Computational Chemistry*, **2017**, 38, 781-789	3.5	47
85	Selectivity for CO2 over CH4 on a functionalized periodic mesoporous phenylene-silica explained by transition state theory. *Chemical Physics Letters*, **2017**, 671, 161-164	2.5	12
84	Functionalization of graphyne by transition metal adatoms. *Carbon*, **2017**, 120, 63-70	10.4	55
83	Effective and Highly Selective CO Generation from CO2 Using a Polycrystalline Mo2C Catalyst. *ACS Catalysis*, **2017**, 7, 4323-4335	13.1	68
82	Highly active Au/MoC and Au/Mo2C catalysts for the low-temperature water gas shift reaction: effects of the carbide metal/carbon ratio on the catalyst performance. *Catalysis Science and Technology*, **2017**, 7, 5332-5342	5.5	26
81	Cohesion and coordination effects on transition metal surface energies. *Surface Science*, **2017**, 664, 45-49	1.8	15
80	ZnO powders as multi-facet single crystals. *Physical Chemistry Chemical Physics*, **2017**, 19, 10622-10628	3.6	10
79	Predicting core level binding energies shifts: Suitability of the projector augmented wave approach as implemented in VASP. *Journal of Computational Chemistry*, **2017**, 38, 518-522	3.5	34
78	Bandgap engineering by cationic disorder: case study on AgBiS. *Physical Chemistry Chemical Physics*, **2017**, 19, 27940-27944	3.6	16
77	Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials. *Nature Communications*, **2017**, 8, 1957	17.4	38

76	Size dependent structural and polymorphic transitions in ZnO: from nanocluster to bulk. *Nanoscale*, **2017**, 9, 10067-10074	7.7	42
75	Substrate-mediated single-atom isolation: dispersion of Ni and La on graphyne. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	9
74	Adsorption and dissociation of molecular hydrogen on orthorhombic Mo2C and cubic MoC (001) surfaces. *Surface Science*, **2017**, 656, 24-32	1.8	34
73	The contact of graphene with Ni(111) surface: description by modern dispersive forces approaches. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	14
72	Highly Active Au/MoC and Cu/MoC Catalysts for the Conversion of CO2: The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability. *Journal of the American Chemical Society*, **2016**, 138, 8269-78	16.4	92
71	Transition metal carbides as novel materials for CO2 capture, storage, and activation. *Energy and Environmental Science*, **2016**, 9, 141-144	35.4	115
70	Performance of Minnesota functionals on predicting core-level binding energies of molecules containing main-group elements. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	16
69	The conversion of CO2 to methanol on orthorhombic Mo2C and Cu/Mo2C catalysts: mechanism for admetal induced change in the selectivity and activity. *Catalysis Science and Technology*, **2016**, 6, 6766-6777	5.5	74
68	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. *Journal of Chemical Theory and Computation*, **2016**, 12, 324-31	6.4	32
67	On the hydrogen adsorption and dissociation on Cu surfaces and nanorows. *Surface Science*, **2016**, 646, 221-229	1.8	25
66	Matildite versus schapbachite: First-principles investigation of the origin of photoactivity in AgBiS2. *Physical Review B*, **2016**, 94,	3.3	29
65	Effect of the Exchange-Correlation Potential on the Transferability of Brønsted-Evans-Polanyi Relationships in Heterogeneous Catalysis. *Journal of Chemical Theory and Computation*, **2016**, 12, 2121-6	6.4	15
64	Morphology effects in photoactive ZnO nanostructures: photooxidative activity of polar surfaces. *Journal of Materials Chemistry A*, **2015**, 3, 8782-8792	13	31
63	Electronic-structure-based material descriptors: (in)dependence on self-interaction and Hartree-Fock exchange. *Chemical Communications*, **2015**, 51, 5602-5	5.8	17
62	Structure and electronic properties of Cu nanoclusters supported on Mo2C(001) and MoC(001) surfaces. *Journal of Chemical Physics*, **2015**, 143, 114704	3.9	22
61	Transition metal adatoms on graphene: A systematic density functional study. *Carbon*, **2015**, 95, 525-534	10.4	103
60	Fundamentals of Methanol Synthesis on Metal Carbide Based Catalysts: Activation of CO2 and H2. *Topics in Catalysis*, **2015**, 58, 159-173	2.3	50
59	Methane capture at room temperature: adsorption on cubic MoC and orthorhombic Mo2C molybdenum carbide (001) surfaces. *RSC Advances*, **2015**, 5, 33737-33746	3.7	14

58	Understanding the reactivity of metallic nanoparticles: beyond the extended surface model for catalysis. *Chemical Society Reviews*, **2014**, 43, 4922-39	58.5	132
57	Hydroxyl Identification on ZnO by Infrared Spectroscopies: Theory and Experiments. *Journal of Physical Chemistry C*, **2014**, 118, 1492-1505	3.8	33
56	Hydrogen storage on metal oxide model clusters using density-functional methods and reliable van der Waals corrections. *Physical Chemistry Chemical Physics*, **2014**, 16, 5382-92	3.6	21
55	Vacancy patterning and patterning vacancies: controlled self-assembly of fullerenes on metal surfaces. *Nanoscale*, **2014**, 6, 10850-8	7.7	5
54	The bending machine: CO2 activation and hydrogenation on δMoC(001) and βMo2C(001) surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 14912-21	3.6	131
53	Ionic Liquid Chiral Resolution: Methyl 2-Ammonium Chloride Propanoate on Al(854)S Surface. *Journal of Physical Chemistry C*, **2014**, 118, 1568-1575	3.8	2
52	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3832-9	6.4	187
51	A DF-vdW study of the CH4 adsorption on different Ni surfaces. *Surface Science*, **2014**, 625, 64-68	1.8	21
50	When reconstruction comes around: Ni, Cu, and Au adatoms on δMoC(001). *Surface Science*, **2014**, 624, 32-36	1.8	5
49	Charge Polarization at a Au–TiC Interface and the Generation of Highly Active and Selective Catalysts for the Low-Temperature Water–Gas Shift Reaction. *Angewandte Chemie*, **2014**, 126, 11452-11456	3.6	8
48	Charge polarization at a Au-TiC interface and the generation of highly active and selective catalysts for the low-temperature water-gas shift reaction. *Angewandte Chemie - International Edition*, **2014**, 53, 11270-4	16.4	54
47	Theoretical assessment of graphene-metal contacts. *Journal of Chemical Physics*, **2013**, 138, 244701	3.9	53
46	Atomic and electronic structure of molybdenum carbide phases: bulk and low Miller-index surfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 12617-25	3.6	151
45	Tuning the surface chemistry of Pd by atomic C and H: a microscopic picture. *Chemistry - A European Journal*, **2013**, 19, 1335-45	4.8	26
44	Brønsted–Evans–Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 4168-4171	3.8	56
43	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. *Journal of Chemical Theory and Computation*, **2013**, 9, 1631-40	6.4	153
42	Microscopic origin of n-type behavior in Si-doped AlN. *Physical Review B*, **2013**, 88,	3.3	15
41	Influence of the surface dipole layer and Pauli repulsion on band energies and doping in graphene adsorbed on metal surfaces. *Physical Review B*, **2012**, 86,	3.3	33

40	Growth and electronic structure of nitrogen-doped graphene on Ni(111). *Physical Review B*, **2012**, 86,	3.3	73
39	Bonding Mechanisms of Graphene on Metal Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 7360-7368	4.8	121
38	Formation of one-dimensional electronic states along the step edges of CeO2(111). *ACS Nano*, **2012**, 6, 1126-33	16.7	55
37	Absolute Surface Step Energies: Accurate Theoretical Methods Applied to Ceria Nanoislands. *Journal of Physical Chemistry Letters*, **2012**, 3, 1956-1961	6.4	35
36	Competition for graphene: graphynes with direction-dependent Dirac cones. *Physical Review Letters*, **2012**, 108, 086804	7.4	809
35	On the interaction of polycyclic aromatic compounds with graphene. *Carbon*, **2012**, 50, 2482-2492	10.4	61
34	Kinetics of the sulfur oxidation on palladium: a combined in situ x-ray photoelectron spectroscopy and density-functional study. *Journal of Chemical Physics*, **2012**, 136, 094702	3.9	18
33	Nanoscale thermal stabilization via permutational premelting. *Physical Review B*, **2012**, 85,	3.3	11
32	Graphene on Ni(111): Coexistence of Different Surface Structures. *Journal of Physical Chemistry Letters*, **2011**, 2, 759-764	6.4	139
31	Adsorption and reaction of SO2 on clean and oxygen precovered Pd(100)--a combined HR-XPS and DF study. *Physical Chemistry Chemical Physics*, **2011**, 13, 16227-35	3.6	17
30	SO2 Adsorption on Pt(111) and Oxygen Precovered Pt(111): A Combined Infrared Reflection Absorption Spectroscopy and Density Functional Study. *Journal of Physical Chemistry C*, **2011**, 115, 479-491	4.8	53
29	Bandgap engineering of graphene by physisorbed adsorbates. *Advanced Materials*, **2011**, 23, 2638-43	24	75
28	Template-Assisted Formation of Fullerenes from Short-Chain Hydrocarbons by Supported Platinum Nanoparticles. *Angewandte Chemie*, **2011**, 123, 4707-4710	3.6	
27	Template-assisted formation of fullerenes from short-chain hydrocarbons by supported platinum nanoparticles. *Angewandte Chemie - International Edition*, **2011**, 50, 4611-4	16.4	9
26	Novel Au/TiC catalysts for CO oxidation and desulfurization processes. *Catalysis Today*, **2011**, 166, 2-9	5.3	35
25	Density Functional Calculations and IR Reflection Absorption Spectroscopy on the Interaction of SO2 with Oxide-Supported Pd Nanoparticles. *Journal of Physical Chemistry C*, **2010**, 114, 13813-13824	3.8	18
24	Desulfurization Reactions on Surfaces of Metal Carbides: Photoemission and Density Functional Studies. *Topics in Catalysis*, **2010**, 53, 393-402	2.3	24
23	Methane activation by platinum: critical role of edge and corner sites of metal nanoparticles. *Chemistry - A European Journal*, **2010**, 16, 6530-9	4.8	112

22	Role of C and P Sites on the Chemical Activity of Metal Carbides and Phosphides: From Clusters to Single-Crystal Surfaces **2010**, 117-132		3
21	Edge sites as a gate for subsurface carbon in palladium nanoparticles. *Journal of Catalysis*, **2009**, 266, 59-63	7.3	64
20	Desulfurization of thiophene on Au/TiC(001): Au-C interactions and charge polarization. *Journal of the American Chemical Society*, **2009**, 131, 8595-602	16.4	64
19	Effect of the Support on the Electronic Structure of Au Nanoparticles Supported on Transition Metal Carbides: Choice of the Best Substrate for Au Activation. *Journal of Physical Chemistry C*, **2009**, 113, 19994-20001	3.8	23
18	Adsorption and diffusion of Au atoms on the (001) surface of Ti, Zr, Hf, V, Nb, Ta, and Mo carbides. *Journal of Chemical Physics*, **2009**, 130, 244706	3.9	15
17	Carbon on platinum substrates: from carbidic to graphitic phases on the (111) surface and on nanoparticles. *Journal of Physical Chemistry A*, **2009**, 113, 11963-73	2.8	41
16	Catalyst size matters: Tuning the molecular mechanism of the water gas shift reaction on titanium carbide based compounds. *Journal of Catalysis*, **2008**, 260, 103-112	7.3	67
15	A Combined Density-Functional and IRAS Study on the Interaction of NO with Pd Nanoparticles: Identifying New Adsorption Sites with Novel Properties. *Journal of Physical Chemistry C*, **2008**, 112, 16539-16549	3.8	38
14	Density functional calculations of Pd nanoparticles using a plane-wave method. *Journal of Physical Chemistry A*, **2008**, 112, 8911-5	2.8	40
13	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. *Theoretical Chemistry Accounts*, **2008**, 120, 565-573	1.9	56
12	Dissociation of SO2 on Au/TiC(001): effects of Au-C interactions and charge polarization. *Angewandte Chemie - International Edition*, **2008**, 47, 6685-9	16.4	64
11	Dissociation of SO2 on Au/TiC(001): Effects of Au–C Interactions and Charge Polarization. *Angewandte Chemie*, **2008**, 120, 6787-6791	3.6	17
10	Density Functional Study of the Adsorption of Atomic Oxygen on the (001) Surface of Early Transition-Metal Carbides. *Journal of Physical Chemistry C*, **2007**, 111, 1307-1314	3.8	61
9	A Systematic Density Functional Study of Molecular Oxygen Adsorption and Dissociation on the (001) Surface of Group IV–VI Transition Metal Carbides. *Journal of Physical Chemistry C*, **2007**, 111, 16982-16989	3.8	58
8	Adsorption of gold on TiC(001): Au-C interactions and charge polarization. *Journal of Chemical Physics*, **2007**, 127, 211102	3.9	59
7	On the mechanism of formation of metal nanowires by self-assembly. *Angewandte Chemie - International Edition*, **2007**, 46, 7094-7	16.4	48
6	On the Mechanism of Formation of Metal Nanowires by Self-Assembly. *Angewandte Chemie*, **2007**, 119, 7224-7227	3.6	6
5	Role of kinetics in the selective surface oxidations of transition metal carbides. *Journal of Physical Chemistry B*, **2006**, 110, 15454-8	3.4	29

4	The interaction of CO2 with sodium-promoted W(011). *Physical Chemistry Chemical Physics*, **2005**, 7, 3866-73	3.6	17
3	A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides. *Journal of Chemical Physics*, **2005**, 122, 174709	3.9	157
2	Interaction of oxygen with ZrC(001) and VC(001): Photoemission and first-principles studies. *Physical Review B*, **2005**, 72,	3.3	40
1	Thermodynamics and Kinetics of Molecular Hydrogen Adsorption and Dissociation on MXenes: Relevance to Heterogeneously Catalyzed Hydrogenation Reactions. *ACS Catalysis*,12850-12857	13.1	4