Gianfranco Pacchioni

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596 papers	32,034 citations	90 h-index	151 g-index
638 ext. papers	34,201 ext. citations	5.1 avg, IF	7.61 L-index

#	Paper	IF	Citations
596	Characterization of paramagnetic species in N-doped TiO2 powders by EPR spectroscopy and DFT calculations. *Journal of Physical Chemistry B*, **2005**, 109, 11414-9	3.4	847
595	N-doped TiO2: Theory and experiment. *Chemical Physics*, **2007**, 339, 44-56	2.3	766
594	Origin of photoactivity of nitrogen-doped titanium dioxide under visible light. *Journal of the American Chemical Society*, **2006**, 128, 15666-71	16.4	761
593	Theory of Carbon Doping of Titanium Dioxide. *Chemistry of Materials*, **2005**, 17, 6656-6665	9.6	614
592	Reduced and n-Type Doped TiO2: Nature of Ti3+ Species. *Journal of Physical Chemistry C*, **2009**, 113, 20543-20552	4.8	572
591	Electronic structure of defect states in hydroxylated and reduced rutile TiO2(110) surfaces. *Physical Review Letters*, **2006**, 97, 166803	7.4	542
590	Origin of the different photoactivity of N-doped anatase and rutile TiO2. *Physical Review B*, **2004**, 70,	3.3	477
589	Oxide ultra-thin films on metals: new materials for the design of supported metal catalysts. *Chemical Society Reviews*, **2008**, 37, 2224-42	58.5	459
588	Excess electron states in reduced bulk anatase TiO2: comparison of standard GGA, GGA+U, and hybrid DFT calculations. *Journal of Chemical Physics*, **2008**, 129, 154113	3.9	429
587	Increasing Oxide Reducibility: The Role of Metal/Oxide Interfaces in the Formation of Oxygen Vacancies. *ACS Catalysis*, **2017**, 7, 6493-6513	13.1	375
586	Acetylene Cyclotrimerization on Supported Size-Selected Pdn Clusters (1≤n≤30): One Atom Is Enough!. *Journal of the American Chemical Society*, **2000**, 122, 3453-3457	16.4	355
585	Oxygen vacancy: the invisible agent on oxide surfaces. *ChemPhysChem*, **2003**, 4, 1041-7	3.2	353
584	Charging of metal atoms on ultrathin MgO/Mo(100) films. *Physical Review Letters*, **2005**, 94, 226104	7.4	324
583	Control of the charge state of metal atoms on thin MgO films. *Physical Review Letters*, **2007**, 98, 096107	7.4	296
582	The Nature of Defects in Fluorine-Doped TiO2. *Journal of Physical Chemistry C*, **2008**, 112, 8951-8956	3.8	293
581	Ab Initio Cluster Model Calculations on the Chemisorption of CO2 and SO2 Probe Molecules on MgO and CaO (100) Surfaces. A Theoretical Measure of Oxide Basicity. *Journal of the American Chemical Society*, **1994**, 116, 10152-10158	16.4	274
580	Bonding trends and dimensionality crossover of gold nanoclusters on metal-supported MgO thin films. *Physical Review Letters*, **2006**, 97, 036106	7.4	261

579	Mechanisms responsible for chemical shifts of core-level binding energies and their relationship to chemical bonding. *Journal of Electron Spectroscopy and Related Phenomena*, **1999**, 100, 215-236	1.7	254
578	Systematic Density Functional Study of the Adsorption of Transition Metal Atoms on the MgO(001) Surface. *Journal of Physical Chemistry B*, **1997**, 101, 2786-2792	3.4	252
577	Structural evolution of atomically dispersed Pt catalysts dictates reactivity. *Nature Materials*, **2019**, 18, 746-751	27	250
576	Trends in non-metal doping of anatase TiO2: B, C, N and F. *Catalysis Today*, **2013**, 206, 12-18	5.3	238
575	Electron transfer at oxide surfaces. The MgO paradigm: from defects to ultrathin films. *Chemical Reviews*, **2013**, 113, 4035-72	68.1	232
574	Theoretical description of hole localization in a quartz Al center: The importance of exact electron exchange. *Physical Review B*, **2000**, 63,	3.3	230
573	Tuning the surface metal work function by deposition of ultrathin oxide films: Density functional calculations. *Physical Review B*, **2006**, 73,	3.3	221
572	Electronic Structure of F and V Centers on the MgO Surface. *The Journal of Physical Chemistry*, **1995**, 99, 17010-17018		214
571	Doping of WO3 for Photocatalytic Water Splitting: Hints from Density Functional Theory. *Journal of Physical Chemistry C*, **2012**, 116, 8901-8909	3.8	206
570	Molecular orbital cluster model study of bonding and vibrations of CO adsorbed on MgO surface. *International Journal of Quantum Chemistry*, **1992**, 42, 1115-1139	2.1	206
569	Electronic and Structural Properties of WO3: A Systematic Hybrid DFT Study. *Journal of Physical Chemistry C*, **2011**, 115, 8345-8353	3.8	200
568	Modeling doped and defective oxides in catalysis with density functional theory methods: room for improvements. *Journal of Chemical Physics*, **2008**, 128, 182505	3.9	195
567	Silicon and germanium clusters. A theoretical study of their electronic structures and properties. *Journal of Chemical Physics*, **1986**, 84, 3301-3310	3.9	185
566	The interplay between structure and CO oxidation catalysis on metal-supported ultrathin oxide films. *Angewandte Chemie - International Edition*, **2010**, 49, 4418-21	16.4	178
565	Density Functional Theory and Electron Paramagnetic Resonance Study on the Effect of N□ Codoping of TiO2. *Chemistry of Materials*, **2008**, 20, 3706-3714	9.6	178
564	Ab initio theory of optical transitions of point defects in SiO2. *Physical Review B*, **1998**, 57, 818-832	3.3	174
563	Electronic interactions and charge transfers of metal atoms and clusters on oxide surfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 1737-57	3.6	171
562	Work function changes induced by deposition of ultrathin dielectric films on metals: A theoretical analysis. *Physical Review B*, **2008**, 78,	3.3	162

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560	QUANTUM CHEMISTRY OF OXIDE SURFACES: FROM CO CHEMISORPTION TO THE IDENTIFICATION OF THE STRUCTURE AND NATURE OF POINT DEFECTS ON MgO. *Surface Review and Letters*, **2000**, 07, 277-306	1.1	161
559	Metal Deposition on Oxide Surfaces: A Quantum-Chemical Study of the Interaction of Rb, Pd, and Ag Atoms with the Surface Vacancies of MgO. *The Journal of Physical Chemistry*, **1996**, 100, 9032-9037		161
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557	Supported nickel and copper clusters on MgO(100): A first-principles calculation on the metal/oxide interface. *Journal of Chemical Physics*, **1996**, 104, 7329-7337	3.9	151
556	Boron-Doped Anatase TiO2: Pure and Hybrid DFT Calculations. *Journal of Physical Chemistry C*, **2009** , 113, 220-228	3.8	146
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552	Oxide films at the nanoscale: new structures, new functions, and new materials. *Accounts of Chemical Research*, **2011**, 44, 1244-52	24.3	141
551	Electronic properties of rutile TiO2 ultrathin films: Odd-even oscillations with the number of layers. *Physical Review B*, **2004**, 70,	3.3	136
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549	Identification of color centers on MgO(001) thin films with scanning tunneling microscopy. *Journal of Physical Chemistry B*, **2006**, 110, 46-9	3.4	133
548	Nature of Ti Interstitials in Reduced Bulk Anatase and Rutile TiO2. *Journal of Physical Chemistry C*, **2009**, 113, 3382-3385	3.8	132
547	Excess electrons stabilized on ionic oxide surfaces. *Accounts of Chemical Research*, **2006**, 39, 861-7	24.3	132
546	Computed Optical Absorption and Photoluminescence Spectra of Neutral Oxygen Vacancies in □Quartz. *Physical Review Letters*, **1997**, 79, 753-756	7.4	130
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544	First Principles Study of Nitrogen Doping at the Anatase TiO2(101) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 9275-9282	3.8	127

543	Paramagnetic defect centers at the MgO surface. An alternative model to oxygen vacancies. *Journal of the American Chemical Society*, **2003**, 125, 738-47	16.4	125
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536	Nature of stable single atom Pt catalysts dispersed on anatase TiO2. *Journal of Catalysis*, **2018**, 367, 104-114	7.3	117
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534	Charging of Au atoms on TiO2 thin films from CO vibrational spectroscopy and DFT calculations. *Journal of Physical Chemistry B*, **2005**, 109, 18418-26	3.4	115
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513	Nucleation of Pd dimers at defect sites of the MgO(100) surface. *Physical Review Letters*, **2004**, 92, 096105	7.4	98
512	Characteristics of Pd adsorption on the MgO(100) surface: Role of oxygen vacancies. *Physical Review B*, **2001**, 64,	3.3	97
511	Controlling the charge state of supported nanoparticles in catalysis: lessons from model systems. *Chemical Society Reviews*, **2018**, 47, 8474-8502	58.5	93
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487	Nature of Ag Islands and Nanoparticles on the CeO2(111) Surface. *Journal of Physical Chemistry C*, **2012**, 116, 1122-1132	3.8	77
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471	Gold and Silver Clusters on TiO2 and ZrO2 (101) Surfaces: Role of Dispersion Forces. *Journal of Physical Chemistry C*, **2015**, 119, 15381-15389	3.8	67
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