

# Marçal Capdevila-Cortada

## List of Publications by Year in descending order

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26  
papers

1,172  
citations

471371

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552653

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g-index

28  
all docs

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docs citations

28  
times ranked

1979  
citing authors

#	ARTICLE	IF	CITATIONS
1	Surface Refaceting Mechanism on Cubic Ceria. Journal of Physical Chemistry Letters, 2020, 11, 7925-7931.	2.1	34
2	Quasi-degenerate states and their dynamics in oxygen deficient reducible metal oxides. Journal of Chemical Physics, 2020, 152, 050901.	1.2	26
3	Dynamic charge and oxidation state of Pt/CeO <sub>2</sub> single-atom catalysts. Nature Materials, 2019, 18, 1215-1221.	13.3	288
4	Mechanism of Ethylene Oxychlorination on Ceria. ACS Catalysis, 2018, 8, 2651-2663.	5.5	22
5	Understanding room-temperature $\ddot{\text{C}}\text{-dimerisation}$ of radical ions: intramolecular $\ddot{\text{C}}\text{-[TTF]}_{2+}$ in functionalised calix[4]arenes. Physical Chemistry Chemical Physics, 2017, 19, 3807-3819.	1.3	7
6	Semihydrogenation of Acetylene on Indium Oxide: Proposed Single-Ensemble Catalysis. Angewandte Chemie, 2017, 129, 10895-10900.	1.6	17
7	Semihydrogenation of Acetylene on Indium Oxide: Proposed Single-Ensemble Catalysis. Angewandte Chemie - International Edition, 2017, 56, 10755-10760.	7.2	82
8	Entropic contributions enhance polarity compensation for CeO <sub>2</sub> (100) surfaces. Nature Materials, 2017, 16, 328-334.	13.3	88
9	Formation of Long, Multicenter $\ddot{\text{C}}\text{-[TCNE]}_{2+}$ Dimers in Solution: Solvation and Stability Assessed through Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 17037-17046.	1.7	7
10	The Tetracyanopyridinide Dimer Dianion, $\ddot{\text{C}}\text{-[TCNPy]}_{2-}$ . Chemistry - A European Journal, 2016, 22, 12312-12315.	1.7	3
11	Performance of DFT+U Approaches in the Study of Catalytic Materials. ACS Catalysis, 2016, 6, 8370-8379.	5.5	135
12	Reactivity descriptors for ceria in catalysis. Applied Catalysis B: Environmental, 2016, 197, 299-312.	10.8	112
13	Orientalional Preference of Long, Multicenter Bonds in Radical Anion Dimers: A Case Study of $\ddot{\text{C}}\text{-[TCNB]}_{2+}$ and $\ddot{\text{C}}\text{-[TCNP]}_{2+}$ . Chemistry - A European Journal, 2015, 21, 6420-6432.	1.7	14
14	Electronic Excitation Energies in Dimers between Radical Ions Presenting Long, Multicenter Bonding. Journal of Chemical Theory and Computation, 2015, 11, 2651-2660.	2.3	6
15	The nature of the $\text{C}\cdots\text{Br}\cdots\text{C}$ intermolecular interactions found in molecular crystals: a general theoretical-database study. CrystEngComm, 2015, 17, 3354-3365.	1.3	32
16	Unraveling the structure sensitivity in methanol conversion on CeO <sub>2</sub> : A DFT+U study. Journal of Catalysis, 2015, 327, 58-64.	3.1	91
17	Descriptor Analysis in Methanol Conversion on Doped CeO <sub>2</sub> (111): Guidelines for Selectivity Tuning. ACS Catalysis, 2015, 5, 6473-6480.	5.5	30
18	Multistep $\ddot{\text{C}}\text{-Dimerization}$ of Tetrakis( $n$ -decyl)heptathienoacene Radical Cations: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2014, 20, 10351-10359.	1.7	12

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19	The nature of the C <sup>+</sup> ⋯Cl <sup>-</sup> ⋯C intermolecular interactions found in molecular crystals: a general theoretical-database study covering the 2.75–4.0 Å... range. <i>CrystEngComm</i> , 2014, 16, 8232-8242.	1.3	34
20	Assessing the Performance of CASPT2 and DFT Methods for the Description of Long, Multicenter Bonding in Dimers between Radical Ions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 650-658.	2.3	29
21	Structure and Properties of Nitrogen-Rich 1,4-Dicyanotetrazine, C <sub>4</sub> N <sub>6</sub> : A Comparative Study with Related Tetracyano Electron Acceptors. <i>Journal of Organic Chemistry</i> , 2014, 79, 8189-8201.	1.7	5
22	The Origin of the Room-Temperature Stability of [TTF] <sub>2</sub> <sup>+</sup> ⋯[TTF] <sub>2</sub> <sup>-</sup> Long, Multicenter Bonds Found in Functionalized [R-TTF] <sub>2</sub> <sup>+</sup> Dimers Included in the Cucurbit[8]uril Cavity. <i>Chemistry - A European Journal</i> , 2014, 20, 7784-7795.	1.7	12
23	Keys for the Existence of Stable Dimers of Bis-tetrathiafulvalene (bis-TTF)-Functionalized Molecular Clips Presenting [TTF] <sup>+</sup> ⋯[TTF] <sup>-</sup> Long, Multicenter Bonds at Room Temperature. <i>Journal of the American Chemical Society</i> , 2013, 135, 13814-13826.	6.6	30
24	The Nature of the [TTF] <sup>+</sup> ⋯[TTF] <sup>-</sup> Interactions in the [TTF] <sub>2</sub> <sup>+</sup> Dimers Embedded in Charged [3]Catenanes: Room-Temperature Multicenter Long Bonds. <i>Chemistry - A European Journal</i> , 2012, 18, 5335-5344.	1.7	22
25	Substituent and counterion effects on the formation of [TTF] <sub>2</sub> <sup>+</sup> dimer dications of end-capped heptathienoacenes. <i>Chemical Communications</i> , 2011, 47, 12622.	2.2	14
26	Unusually Long, Multicenter, Cation <sup>+</sup> ⋯Anion <sup>-</sup> Bonding Observed for Several Polymorphs of [TTF] <sub>2</sub> [TCNE]. <i>Chemistry - A European Journal</i> , 2011, 17, 9326-9341.	1.7	18