Andrea Martini

List of Publications by Year
in descending order

40 papers	1,463 citations	430874 18 h-index	330143 37 g-index
40 all docs	40 docs citations	40 times ranked	1334 citing authors

#	Article	IF	Citations
1	SO₂ Poisoning of Cu-CHA deNO_x Catalyst: The Most Vulnerable Cu Species Identified by X-ray Absorption Spectroscopy. Jacs Au, 2022, 2, 787-792.	7.9	10
2	Assessing the Influence of Zeolite Composition on Oxygen-Bridged Diamino Dicopper(II) Complexes in Cu-CHA DeNO_x Catalysts by Machine Learning-Assisted X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 6164-6170.	4.6	10
3	Cu- and Fe-speciation in a composite zeolite catalyst for selective catalytic reduction of NO_x: insights from operando XAS. Catalysis Science and Technology, 2021, 11, 846-860.	4.1	8
4	Direct structural and mechanistic insights into fast bimolecular chemical reactions in solution through a coupled XAS/UVâ€“Vis multivariate statistical analysis. Dalton Transactions, 2021, 50, 131-142.	3.3	10
5	Activation of Câ€“H bonds by a nonheme iron(iv)â€“oxo complex: mechanistic evidence through a coupled EDXAS/UV-Vis multivariate analysis. Physical Chemistry Chemical Physics, 2021, 23, 1188-1196.	2.8	9
6	Quantitative Analysis of the UVâ€“Vis Spectra for Gold Nanoparticles Powered by Supervised Machine Learning. Journal of Physical Chemistry C, 2021, 125, 8656-8666.	3.1	19
7	Electronic Properties of Ti Sites in Zieglerâ€“Natta Catalysts. ACS Catalysis, 2021, 11, 9949-9961.	11.2	32
8	Revisiting the Extended X-ray Absorption Fine Structure Fitting Procedure through a Machine Learning-Based Approach. Journal of Physical Chemistry A, 2021, 125, 7080-7091.	2.5	15
9	Copper Pairing in the Mordenite Framework as a Function of the Cu^I/Cu^{II} Speciation. Angewandte Chemie - International Edition, 2021, 60, 25891-25896.	13.8	16
10	Investigating the role of Cu-oxo species in Cu-nitrate formation over Cu-CHA catalysts. Physical Chemistry Chemical Physics, 2021, 23, 18322-18337.	2.8	14
11	In situ X-ray absorption study of Cu species in Cu-CHA catalysts for NH3-SCR during temperature-programmed reduction in NO/NH3. Research on Chemical Intermediates, 2021, 47, 357-375.	2.7	7
12	Machine learning powered by principal component descriptors as the key for sorted structural fit of XANES. Physical Chemistry Chemical Physics, 2021, 23, 17873-17887.	2.8	7
13	Insights into the Structure of Reaction Intermediates Through Coupled X-ray Absorption/UV-Vis Spectroscopy. Springer Proceedings in Physics, 2021, , 141-154.	0.2	5
14	Estimating a Set of Pure XANES Spectra from Multicomponent Chemical Mixtures Using a Transformation Matrix-Based Approach. Springer Proceedings in Physics, 2021, , 65-84.	0.2	7
15	Search for Analytical Relations between X-Ray Absorption Spectra Descriptors and the Local Atomic Structure Using Machine Learning. Journal of Surface Investigation, 2021, 15, 934-938.	0.5	5
16	Understanding X-ray absorption spectra by means of descriptors and machine learning algorithms. Npj Computational Materials, 2021, 7, .	8.7	48
17	Local structure of Cu(I) ions in the MOR zeolite: A DFT-assisted XAS study. Radiation Physics and Chemistry, 2020, 175, 108111.	2.8	7
18	Wavelet analysis of a Cu-oxo zeolite EXAFS simulated spectrum. Radiation Physics and Chemistry, 2020, 175, 108333.	2.8	7

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19	Identifying Cu-oxo species in Cu-zeolites by XAS: A theoretical survey by DFT-assisted XANES simulation and EXAFS wavelet transform. Catalysis Today, 2020, 345, 125-135.	4.4	68
20	DFT-assisted XANES simulations to discriminate different monomeric CuII species in CHA catalysts. Radiation Physics and Chemistry, 2020, 175, 108510.	2.8	3
21	Machine learning approaches to XANES spectra for quantitative 3D structural determination: The case of CO2 adsorption on CPO-27-Ni MOF. Radiation Physics and Chemistry, 2020, 175, 108430.	2.8	21
22	PyFitit: The software for quantitative analysis of XANES spectra using machine-learning algorithms. Computer Physics Communications, 2020, 250, 107064.	7.5	64
23	Bridging Solution and Solid-State Chemistry of Dicyanoaurate: The Case Study of Znâ€“Au Nucleation Units. Inorganic Chemistry, 2020, 59, 203-213.	4.0	17
24	Spectral Decomposition of X-ray Absorption Spectroscopy Datasets: Methods and Applications. Crystals, 2020, 10, 664.	2.2	22
25	Structure and Reactivity of Oxygen-Bridged Diamino Dicopper(II) Complexes in Cu-Ion-Exchanged Chabazite Catalyst for NH₃-Mediated Selective Catalytic Reduction. Journal of the American Chemical Society, 2020, 142, 15884-15896.	13.7	110
26	EXAFS wavelet transform analysis of Cu-MOR zeolites for the direct methane to methanol conversion. Physical Chemistry Chemical Physics, 2020, 22, 18950-18963.	2.8	35
27	Direct Mechanistic Evidence for a Nonheme Complex Reaction through a Multivariate XAS Analysis. Inorganic Chemistry, 2020, 59, 9979-9989.	4.0	13
28	THORONDOR: a software for fast treatment and analysis of low-energy XAS data. Journal of Synchrotron Radiation, 2020, 27, 1741-1752.	2.4	12
29	Cu-Exchanged Ferrierite Zeolite for the Direct CH4 to CH3OH Conversion: Insights on Cu Speciation from X-Ray Absorption Spectroscopy. Topics in Catalysis, 2019, 62, 712-723.	2.8	9
30	Glutathione activation of an organometallic half-sandwich anticancer drug candidate by ligand attack. Chemical Communications, 2019, 55, 14602-14605.	4.1	21
31	Quantitative structural determination of active sites from in situ and operando XANES spectra: From standard ab initio simulations to chemometric and machine learning approaches. Catalysis Today, 2019, 336, 3-21.	4.4	70
32	Understanding and Optimizing the Performance of Cuâ€FER for The Direct CH₄ to CH₃OH Conversion. ChemCatChem, 2019, 11, 621-627.	3.7	29
33	The impact of reaction conditions and material composition on the stepwise methane to methanol conversion over Cu-MOR: An operando XAS study. Catalysis Today, 2019, 336, 99-108.	4.4	26
34	The Nuclearity of the Active Site for Methane to Methanol Conversion in Cu-Mordenite: A Quantitative Assessment. Journal of the American Chemical Society, 2018, 140, 15270-15278.	13.7	177
35	Determining Cuâ€“Speciation in the Cuâ€“CHA Zeolite Catalyst: The Potential of Multivariate Curve Resolution Analysis of In Situ XAS Data. Topics in Catalysis, 2018, 61, 1396-1407.	2.8	28
36	The insights from X-ray absorption spectroscopy into the local atomic structure and chemical bonding of Metalâ€“organic frameworks. Polyhedron, 2018, 155, 232-253.	2.2	34

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37	Methane to Methanol: Structureâ€“Activity Relationships for Cu-CHA. Journal of the American Chemical Society, 2017, 139, 14961-14975.	13.7	277
38	The duality of UiO-67-Pt MOFs: connecting treatment conditions and encapsulated Pt species byoperandoXAS. Physical Chemistry Chemical Physics, 2017, 19, 27489-27507.	2.8	28
39	Composition-driven Cu-speciation and reducibility in Cu-CHA zeolite catalysts: a multivariate XAS/FTIR approach to complexity. Chemical Science, 2017, 8, 6836-6851.	7.4	163
40	Copper pairing in the mordenite framework as a function of the Cu(I)/Cu(II) speciation. Angewandte Chemie, 0, , .	2.0	0