Francesco Paesani

List of Publications by Year
in descending order

129	7,644	46984 47	58549 82
papers	citations	h-index	g-index

192	192	192	5837
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient. Journal of Chemical Theory and Computation, 2013, 9, 5395-5403.	2.3	398
2	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. Chemical Reviews, 2016, 116, 7501-7528.	23.0	314
3	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. Journal of Chemical Theory and Computation, 2014, 10, 1599-1607.	2.3	313
4	Development of a â€œFirst-Principlesâ€•Water Potential with Flexible Monomers. III. Liquid Phase Properties. Journal of Chemical Theory and Computation, 2014, 10, 2906-2910.	2.3	292
5	On the accuracy of the MB-pol many-body potential for water: Interaction energies, vibrational frequencies, and classical thermodynamic and dynamical properties from clusters to liquid water and ice. Journal of Chemical Physics, 2016, 145, 194504.	1.2	214
6	The Properties of Water: Insights from Quantum Simulations. Journal of Physical Chemistry B, 2009, 113, 5702-5719.	1.2	199
7	An accurate and simple quantum model for liquid water. Journal of Chemical Physics, 2006, 125, 184507.	1.2	187
8	Infrared and Raman Spectroscopy of Liquid Water through â€œFirst-Principlesâ€•Many-Body Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 1145-1154.	2.3	182
9	MIL-101(Fe) as a lithium-ion battery electrode material: a relaxation and intercalation mechanism during lithium insertion. Journal of Materials Chemistry A, 2015, 3, 4738-4744.	5.2	168
10	Dissecting the Molecular Structure of the Air/Water Interface from Quantum Simulations of the Sum-Frequency Generation Spectrum. Journal of the American Chemical Society, 2016, 138, 3912-3919.	6.6	153
11	Proton Transport in a Highly Conductive Porous Zirconiumâ€Based Metalâ€“Organic Framework: Molecular Insight. Angewandte Chemie - International Edition, 2016, 55, 3919-3924.	7.2	152
12	Quantum effects in liquid water from an ab initio-based polarizable force field. Journal of Chemical Physics, 2007, 127, 074506.	1.2	151
13	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. Journal of Chemical Physics, 2018, 148, 241725.	1.2	142
14	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. Journal of Physical Chemistry Letters, 2012, 3, 3765-3769.	2.1	137
15	The Water Hexamer: Cage, Prism, or Both. Full Dimensional Quantum Simulations Say Both. Journal of the American Chemical Society, 2012, 134, 11116-11119.	6.6	132
16	Ice Nucleation Efficiency of Hydroxylated Organic Surfaces Is Controlled by Their Structural Fluctuations and Mismatch to Ice. Journal of the American Chemical Society, 2017, 139, 3052-3064.	6.6	132
17	A Critical Assessment of Two-Body and Three-Body Interactions in Water. Journal of Chemical Theory and Computation, 2013, 9, 1103-1114.	2.3	126
18	Infrared Spectroscopy and Hydrogen-Bond Dynamics of Liquid Water from Centroid Molecular Dynamics with an Ab Initio-Based Force Field. Journal of Physical Chemistry B, 2009, 113, 13118-13130.	1.2	123

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19	Getting the Right Answers for the Right Reasons: Toward Predictive Molecular Simulations of Water with Many-Body Potential Energy Functions. Accounts of Chemical Research, 2016, 49, 1844-1851.	7.6	121
20	Ice-Nucleating and Antifreeze Proteins Recognize Ice through a Diversity of Anchored Clathrate and Ice-like Motifs. Journal of the American Chemical Society, 2018, 140, 4905-4912.	6.6	117
21	Electron affinity of liquid water. Nature Communications, 2018, 9, 247.	5.8	114
22	Preordering of water is not needed for ice recognition by hyperactive antifreeze proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8266-8271.	3.3	89
23	Molecular-Level Characterization of the Breathing Behavior of the Jungle-Gym-type DMOF-1 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2012, 134, 4207-4215.	6.6	87
24	Temperature-dependent vibrational spectra and structure of liquid water from classical and quantum simulations with the MB-pol potential energy function. Journal of Chemical Physics, 2017, 147, 244504.	1.2	87
25	Hydrogen bonding structure of confined water templated by a metal-organic framework with open metal sites. Nature Communications, 2019, 10, 4771.	5.8	86
26	Toward Chemical Accuracy in the Description of Ionâ€“Water Interactions through Many-Body Representations. I. Halideâ€“Water Dimer Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 2698-2705.	2.3	81
27	On the representation of many-body interactions in water. Journal of Chemical Physics, 2015, 143, 104102.	1.2	80
28	A Refined MS-EVB Model for Proton Transport in Aqueous Environments. Journal of Physical Chemistry B, 2012, 116, 343-352.	1.2	79
29	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101.	1.2	74
30	Monitoring Water Clusters â€œMeltâ€•Through Vibrational Spectroscopy. Journal of the American Chemical Society, 2017, 139, 7082-7088.	6.6	69
31	Bulk Contributions Modulate the Sum-Frequency Generation Spectra of Water on Model Sea-Spray Aerosols. CheM, 2018, 4, 1629-1644.	5.8	69
32	Halogen bonding in UiO-66 frameworks promotes superior chemical warfare agent simulant degradation. Chemical Communications, 2019, 55, 3481-3484.	2.2	68
33	Molecular Origin of the Vibrational Structure of Ice I_h. Journal of Physical Chemistry Letters, 2017, 8, 2579-2583.	2.1	66
34	A quantitative assessment of the accuracy of centroid molecular dynamics for the calculation of the infrared spectrum of liquid water. Journal of Chemical Physics, 2010, 132, 014105.	1.2	63
35	Second-Order Vibrational Lineshapes from the Air/Water Interface. Journal of Physical Chemistry A, 2018, 122, 4457-4464.	1.1	63
36	Nuclear Quantum Effects in the Reorientation of Water. Journal of Physical Chemistry Letters, 2010, 1, 2316-2321.	2.1	62

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37	i-TTM Model for Ab Initio-Based Ionâ€“Water Interaction Potentials. 1. Halideâ€“Water Potential Energy Functions. Journal of Physical Chemistry B, 2016, 120, 1822-1832.	1.2	61
38	Many-Body Interactions in Ice. Journal of Chemical Theory and Computation, 2017, 13, 1778-1784.	2.3	60
39	Temperature Dependence of the Air/Water Interface Revealed by Polarization Sensitive Sum-Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 4356-4365.	1.2	59
40	Toward chemical accuracy in the description of ionâ€“water interactions through many-body representations. Alkali-water dimer potential energy surfaces. Journal of Chemical Physics, 2017, 147, 161715.	1.2	57
41	Pore Breathing of Metalâ€“Organic Frameworks by Environmental Transmission Electron Microscopy. Journal of the American Chemical Society, 2017, 139, 13973-13976.	6.6	56
42	Ion-mediated hydrogen-bond rearrangement through tunnelling in the iodideâ€“dihydrate complex. Nature Chemistry, 2019, 11, 367-374.	6.6	55
43	Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems. Journal of Chemical Theory and Computation, 2012, 8, 2868-2877.	2.3	54
44	Negative Ion Photoelectron Spectroscopy Reveals Thermodynamic Advantage of Organic Acids in Facilitating Formation of Bisulfate Ion Clusters: Atmospheric Implications. Journal of Physical Chemistry Letters, 2013, 4, 779-785.	2.1	53
45	Transmission Electron Microscopy Reveals Deposition of Metal Oxide Coatings onto Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 1348-1357.	6.6	51
46	Engineering the entropy-driven free-energy landscape of a dynamic nanoporous protein assembly. Nature Chemistry, 2018, 10, 732-739.	6.6	51
47	Local superfluidity in inhomogeneous quantum fluids. Physical Review B, 2006, 74, .	1.1	50
48	The end of ice I. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24413-24419.	3.3	50
49	Orientational Distribution of Free O-H Groups of Interfacial Water is Exponential. Physical Review Letters, 2018, 121, 246101.	2.9	49
50	Disentangling Coupling Effects in the Infrared Spectra of Liquid Water. Journal of Physical Chemistry B, 2018, 122, 10754-10761.	1.2	48
51	The effects of electronic polarization on water adsorption in metal-organic frameworks: H2O in MIL-53(Cr). Journal of Chemical Physics, 2012, 137, 054704.	1.2	45
52	Many-Body Effects Determine the Local Hydration Structure of Cs⁺ in Solution. Journal of Physical Chemistry Letters, 2019, 10, 406-412.	2.1	45
53	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	5.8	45
54	Ultrafast direct electron transfer at organic semiconductor and metal interfaces. Science Advances, 2017, 3, e1701508.	4.7	44

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55	Data-Driven Many-Body Models for Molecular Fluids: CO₂/H₂O Mixtures as a Case Study. Journal of Chemical Theory and Computation, 2020, 16, 2246-2257.	2.3	44
56	Water Dynamics in Metalâ€“Organic Frameworks: Effects of Heterogeneous Confinement Predicted by Computational Spectroscopy. Journal of Physical Chemistry Letters, 2014, 5, 2897-2902.	2.1	43
57	The i-TTM model for ab initio-based ionâ€“water interaction potentials. II. Alkali metal ionâ€“water potential energy functions. Physical Chemistry Chemical Physics, 2016, 18, 30334-30343.	1.3	43
58	Molecular Mechanisms of Water-Mediated Proton Transport in MIL-53 Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 19508-19516.	1.5	42
59	Sodiumâ€“carboxylate contact ion pair formation induces stabilization of palmitic acid monolayers at high pH. Physical Chemistry Chemical Physics, 2017, 19, 10481-10490.	1.3	42
60	The curious case of the water hexamer: Cage vs. Prism. Chemical Physics Letters, 2013, 580, 1-8.	1.2	41
61	Molecular Mechanisms of Spin Crossover in the {Fe(pz)[Pt(CN)₄]} Metalâ€“Organic Framework upon Water Adsorption. Journal of the American Chemical Society, 2016, 138, 6123-6126.	6.6	41
62	Computational Exploration of the Water Concentration Dependence of the Proton Transport in the Porous UiOâ€“66(Zr)â€“(CO₂H)₂ Metalâ€“Organic Framework. Chemistry of Materials, 2017, 29, 1569-1576.	3.2	40
63	Vibrational spectra of halide-water dimers: Insights on ion hydration from full-dimensional quantum calculations on many-body potential energy surfaces. Journal of Chemical Physics, 2018, 148, 102321.	1.2	40
64	How good are polarizable and flexible models for water: Insights from a many-body perspective. Journal of Chemical Physics, 2020, 153, 060901.	1.2	39
65	Theoretical Modeling of Spin Crossover in Metalâ€“Organic Frameworks: [Fe(pz)₂Pt(CN)₄] as a Case Study. Inorganic Chemistry, 2014, 53, 11020-11028.	1.9	38
66	Assessing Many-Body Effects of Water Self-Ions. I: OH^{â€“}(H₂O)_n Clusters. Journal of Chemical Theory and Computation, 2018, 14, 1982-1997.	2.3	38
67	Thermodynamics of Water Dimer Dissociation in the Primary Hydration Shell of the Iodide Ion with Temperature-Dependent Vibrational Predissociation Spectroscopy. Journal of Physical Chemistry A, 2015, 119, 1859-1866.	1.1	37
68	Proton Transport in a Highly Conductive Porous Zirconiumâ€Based Metalâ€“Organic Framework: Molecular Insight. Angewandte Chemie, 2016, 128, 3987-3992.	1.6	37
69	Molecular-Level Interpretation of Vibrational Spectra of Ordered Ice Phases. Journal of Physical Chemistry B, 2018, 122, 10572-10581.	1.2	36
70	Exploring Electrostatic Effects on the Hydrogen Bond Network of Liquid Water through Many-Body Molecular Dynamics. Journal of Physical Chemistry B, 2016, 120, 8539-8546.	1.2	35
71	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. Physical Review Letters, 2018, 121, 137401.	2.9	35
72	Low-order many-body interactions determine the local structure of liquid water. Chemical Science, 2019, 10, 8211-8218.	3.7	35

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73	Halide Ion Microhydration: Structure, Energetics, and Spectroscopy of Small Halideâ€“Water Clusters. Journal of Physical Chemistry A, 2019, 123, 2843-2852.	1.1	35
74	On the interplay of the potential energy and dipole moment surfaces in controlling the infrared activity of liquid water. Journal of Chemical Physics, 2015, 142, 212411.	1.2	33
75	Chemical accuracy in modeling halide ion hydration from many-body representations. Advances in Physics: X, 2019, 4, 1631212.	1.5	32
76	Vaporâ€“liquid equilibrium of water with the MB-pol many-body potential. Journal of Chemical Physics, 2021, 154, 211103.	1.2	32
77	Many-Body Convergence of the Electrostatic Properties of Water. Journal of Chemical Theory and Computation, 2013, 9, 4844-4852.	2.3	29
78	Water in metal-organic frameworks: structure and diffusion of H₂O in MIL-53(Cr) from quantum simulations. Molecular Simulation, 2012, 38, 631-641.	0.9	28
79	General Many-Body Framework for Data-Driven Potentials with Arbitrary Quantum Mechanical Accuracy: Water as a Case Study. Journal of Chemical Theory and Computation, 2021, 17, 5635-5650.	2.3	28
80	Data-Driven Many-Body Models with Chemical Accuracy for CH₄/H₂O Mixtures. Journal of Physical Chemistry B, 2020, 124, 11207-11221.	1.2	28
81	Water Capture Mechanisms at Zeolitic Imidazolate Framework Interfaces. Journal of the American Chemical Society, 2021, 143, 21189-21194.	6.6	28
82	Effects of Surface Pressure on the Properties of Langmuir Monolayers and Interfacial Water at the Airâ€“Water Interface. Langmuir, 2015, 31, 2147-2156.	1.6	27
83	Isomeric Equilibria, Nuclear Quantum Effects, and Vibrational Spectra of M⁺(H₂O)_{n=1â€“3} Clusters, with M = Li, Na, K, Rb, and Cs, through Many-Body Representations. Journal of Physical Chemistry A, 2018, 122, 5811-5821.	1.1	27
84	Spin Crossover in the {Fe(pz)[Pt(CN)₄]} Metalâ€“Organic Framework upon Pyrazine Adsorption. Journal of Physical Chemistry Letters, 2016, 7, 4022-4026.	2.1	26
85	Specific Ion Effects on Hydrogen-Bond Rearrangements in the Halideâ€“Dihydrate Complexes. Journal of Physical Chemistry Letters, 2019, 10, 2823-2828.	2.1	26
86	Nature of Halideâ€“Water Interactions: Insights from Many-Body Representations and Density Functional Theory. Journal of Chemical Theory and Computation, 2019, 15, 2983-2995.	2.3	26
87	Temperature-Dependent Infrared Spectroscopy of Water from a First-Principles Approach. Journal of Physical Chemistry A, 2011, 115, 6861-6871.	1.1	25
88	Neat Waterâ€“Vapor Interface: Proton Continuum and the Nonresonant Background. Journal of Physical Chemistry Letters, 2018, 9, 6744-6749.	2.1	25
89	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model. Journal of Physical Chemistry Letters, 2022, 13, 3652-3658.	2.1	25
90	Guest-Dependent Stabilization of the Low-Spin State in Spin-Crossover Metal-Organic Frameworks. Inorganic Chemistry, 2018, 57, 9839-9843.	1.9	23

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91	Unraveling the effect of defects, domain size, and chemical doping on photophysics and charge transport in covalent organic frameworks. Chemical Science, 2021, 12, 8373-8384.	3.7	23
92	Solvation-Guided Design of Fluorescent Probes for Discrimination of Amyloids. Scientific Reports, 2018, 8, 6950.	1.6	21
93	Relationship between Hydrogen-Bonding Motifs and the 1b₁ Splitting in the X-ray Emission Spectrum of Liquid Water. Journal of Physical Chemistry Letters, 2021, 12, 3996-4002.	2.1	21
94	Data-driven many-body models enable a quantitative description of chloride hydration from clusters to bulk. Journal of Chemical Physics, 2021, 155, 064502.	1.2	21
95	Assessing Many-Body Effects of Water Self-Ions. II: H₃O⁺(H₂O)_n Clusters. Journal of Chemical Theory and Computation, 2019, 15, 4816-4833.	2.3	20
96	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartreeâ€“Fock Density?. Journal of Chemical Theory and Computation, 2022, 18, 4745-4761.	2.3	20
97	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. Journal of Chemical Theory and Computation, 2019, 15, 2359-2374.	2.3	18
98	Computer simulations explain mutation-induced effects on the DNA editing by adenine base editors. Science Advances, 2020, 6, eaaz2309.	4.7	18
99	Active learning of many-body configuration space: Application to the Cs+â€“water MB-nrg potential energy function as a case study. Journal of Chemical Physics, 2020, 152, 144103.	1.2	18
100	MB-Fit: Software infrastructure for data-driven many-body potential energy functions. Journal of Chemical Physics, 2021, 155, 124801.	1.2	18
101	Near- and long-term quantum algorithmic approaches for vibrational spectroscopy. Physical Review A, 2021, 104, .	1.0	17
102	Hydrogen bond dynamics in heavy water studied with quantum dynamical simulations. Physical Chemistry Chemical Physics, 2011, 13, 19865.	1.3	16
103	Nature of Alkali Ionâ€“Water Interactions: Insights from Many-Body Representations and Density Functional Theory. II. Journal of Chemical Theory and Computation, 2020, 16, 3055-3072.	2.3	16
104	Simulation Meets Experiment: Unraveling the Properties of Water in Metalâ€“Organic Frameworks through Vibrational Spectroscopy. Journal of Physical Chemistry C, 2021, 125, 12451-12460.	1.5	16
105	Static and Dynamic Correlations in Water: Comparison of Classical Ab Initio Molecular Dynamics at Elevated Temperature with Path Integral Simulations at Ambient Temperature. Journal of Chemical Theory and Computation, 2022, 18, 2124-2131.	2.3	16
106	Nonlinear quantum time correlation functions from centroid molecular dynamics and the maximum entropy method. Journal of Chemical Physics, 2008, 129, 194113.	1.2	15
107	Infrared signatures of isomer selectivity and symmetry breaking in the Cs+(H2O)3 complex using many-body potential energy functions. Journal of Chemical Physics, 2020, 153, 044306.	1.2	15
108	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. Journal of Chemical Theory and Computation, 2022, 18, 3410-3426.	2.3	14

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109	Highly Accurate Many-Body Potentials for Simulations of N₂O₅ in Water: Benchmarks, Development, and Validation. Journal of Chemical Theory and Computation, 2021, 17, 3931-3945.	2.3	13
110	Assessing the Accuracy of the SCAN Functional for Water through a Many-Body Analysis of the Adiabatic Connection Formula. Journal of Chemical Theory and Computation, 2021, 17, 3739-3749.	2.3	13
111	The effects of framework dynamics on the behavior of water adsorbed in the [Zn(l-L)(Cl)] and Co-MOF-74 metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2016, 18, 8196-8204.	1.3	12
112	Transferability of data-driven, many-body models for CO2 simulations in the vapor and liquid phases. Journal of Chemical Physics, 2022, 156, 104503.	1.2	12
113	Water Structure and Dynamics in Homochiral [Zn(l-L)(X)] Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 18239-18247.	1.5	11
114	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7462-7472.	2.3	11
115	Water is not a dynamic polydisperse branched polymer. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13169-13170.	3.3	10
116	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2020, , 635-660.		10
117	A Ligand Field Molecular Mechanics Study of CO 2 â€Induced Breathing in the Metalâ€“Organic Framework DUTâ€8(Ni). Advanced Theory and Simulations, 2019, 2, 1900098.	1.3	9
118	Rovibrational Spectra for the HCCCNÂ·HCN and HCNÂ·HCCCN Binary Complexes in4He Dropletsâ€. Journal of Physical Chemistry A, 2007, 111, 7516-7528.	1.1	8
119	Water structure at the interface of alcohol monolayers as determined by molecular dynamics simulations and computational vibrational sum-frequency generation spectroscopy. Journal of Chemical Physics, 2019, 150, 034701.	1.2	8
120	Modeling Spontaneous Charge Transfer at Metal/Organic Hybrid Heterostructures. Journal of Physical Chemistry C, 2020, 124, 4802-4809.	1.5	8
121	Density functional theory of water with the machine-learned DM21 functional. Journal of Chemical Physics, 2022, 156, 161103.	1.2	8
122	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. Journal of Chemical Physics, 2022, 157, .	1.2	8
123	Topology-Mediated Enhanced Polaron Coherence in Covalent Organic Frameworks. Journal of Physical Chemistry Letters, 2021, 12, 9442-9448.	2.1	7
124	The behavior of methaneâ€“water mixtures under elevated pressures from simulations using many-body potentials. Journal of Chemical Physics, 2022, 156, .	1.2	7
125	Combined Theoretical, Bioinformatic, and Biochemical Analyses of RNA Editing by Adenine Base Editors. CRISPR Journal, 2022, 5, 294-310.	1.4	4
126	Analytical STEM Investigation of the Post-Synthetic Modification (PMS) of Metal-Organic Frameworks (MOFs): Metal- and Ligand-Exchange in UiO-66. Microscopy and Microanalysis, 2018, 24, 1970-1971.	0.2	3

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127	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2018, , 1-25.		2
128	Gas Absorption and Pore Breathing of Metal-Organic Frameworks Studied Using in situ Environmental Transmission Electron Microscopy (ETEM). Microscopy and Microanalysis, 2018, 24, 1880-1881.	0.2	1
129	Sun etÂal. Reply:. Physical Review Letters, 2019, 123, 099602.	2.9	1