

Rui-Zhi Qiu

List of Publications by Year in descending order

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48
papers

690
citations

566801

15
h-index

610482

24
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48
all docs

48
docs citations

48
times ranked

488
citing authors

#	ARTICLE	IF	CITATIONS
1	Insights into the Metal-CO Bond in $O_2M(\dot{I}-CO)$ ($M = Cr, Mo, W, Nd, \text{ and } U$) Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 2066-2075.	1.9	4
2	Matrix-Isolation Infrared Spectra and Electronic Structure Calculations for Dinitrogen Complexes with Uranium Trioxide Molecules $UO_3(\dot{I}-NN)_4$. <i>Inorganic Chemistry</i> , 2022, 61, 11075-11083.	1.9	1
3	New theoretical insights into the actual oxidation states of uranium in the solid-state compounds. <i>Journal of Nuclear Materials</i> , 2021, 543, 152563.	1.3	7
4	Metallic and anti-metallic properties of hydrogen adsorbed AnO_2 ($An = Th, U, \text{ and } Pu$) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 878-885.	1.3	2
5	Low-Temperature CO Oxidation over the Pt-TiN Interfacial Dual Sites. <i>ChemCatChem</i> , 2021, 13, 4610-4617.	1.8	2
6	Revealing the microscopic mechanism of PuO_2 and $\dot{I}\pm Pu_2O_3$ in resisting plutonium hydrogenation via ab initio molecular dynamics simulation. <i>Journal of Alloys and Compounds</i> , 2021, 874, 159904.	2.8	4
7	Hydrogen diffusion in plutonium hydrides from first principles. <i>Journal of Nuclear Materials</i> , 2021, 557, 153247.	1.3	3
8	Theoretical Assignment of Oxidation State of Uranium in Binary, Ternary, and Quaternary Tellurides. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1029-1040.	1.5	2
9	Effective Coulomb interaction in actinides from linear response approach. <i>Computational Materials Science</i> , 2020, 171, 109270.	1.4	14
10	Exploring the sub-stoichiometric behavior of plutonium mononitride. <i>RSC Advances</i> , 2020, 10, 24877-24881.	1.7	3
11	Design, Synthesis and High HER Performances of 3D Ni/Mo Sulfide on Ni Foam. <i>ChemCatChem</i> , 2020, 12, 1647-1652.	1.8	18
12	Diffusion behavior of hydrogen in oxygen saturated and unsaturated plutonium dioxide: An ab initio molecular dynamics study. <i>Journal of Alloys and Compounds</i> , 2020, 834, 155113.	2.8	8
13	Thermodynamical stability of substoichiometric plutonium monocarbide from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9009-9013.	1.3	6
14	Molecular reactions and oxidation corrosion on UN (001) surface under exposure to environment gases: A DFT study. <i>Journal of Nuclear Materials</i> , 2020, 533, 152095.	1.3	5
15	Chemical State of U in $U-Na-O$ Ternary System from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17155-17162.	1.5	9
16	Molecular dynamics simulation studies of displacement cascade induced defects in gold nanotubes. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2019, 461, 142-148.	0.6	0
17	Unraveling the highest oxidation states of actinides in solid-state compounds with a particular focus on plutonium. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4732-4737.	1.3	16
18	Plutonium Oxidation States in Complex Molecular Solids. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12096-12103.	1.5	18

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19	Phase Segregation, Transition, or New Phase Formation of Plutonium Dioxide: The Roles of Transition Metals. <i>Inorganic Chemistry</i> , 2019, 58, 4350-4364.	1.9	21
20	First-principles explorations of the universal picture of oxide layer structure over metallic plutonium. <i>Corrosion Science</i> , 2019, 153, 236-248.	3.0	29
21	Dependency of f states in fluorite-type XO_2 (X = Ce, Th, U) on the stability and electronic state of doped transition metals. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25962-25975.	1.3	10
22	First-Principles Insights into the Oxidation States and Electronic Structures of Ceria-Based Binary, Ternary, and Quaternary Oxides. <i>Journal of Physical Chemistry C</i> , 2019, 123, 175-184.	1.5	10
23	New Insights into the Crystal Structures of Plutonium Hydrides from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10103-10112.	1.5	15
24	Phase transition and intrinsic metric of dipolar fermions in the quantum Hall regime. <i>Physical Review B</i> , 2018, 97, .	1.1	6
25	Light impurity atoms as the probes for the electronic structures of actinide dioxides. <i>Computational Materials Science</i> , 2018, 142, 25-31.	1.4	15
26	Thermodynamical Stability of Plutonium Monoxide with Carbon Substitution. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22821-22828.	1.5	9
27	Density-functional study of plutonium monoxide monohydride. <i>Journal of Nuclear Materials</i> , 2017, 485, 181-188.	1.3	4
28	Structural, mechanical, dynamical and electronic properties and high-pressure behavior of Mo ₂ GeC: A first-principles study. <i>Computational Materials Science</i> , 2017, 137, 306-313.	1.4	7
29	Energetics of intrinsic point defects in aluminium via orbital-free density functional theory. <i>Philosophical Magazine</i> , 2017, 97, 2164-2181.	0.7	18
30	A molecular dynamics simulation study of irradiation induced defects in gold nanowire. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2017, 405, 22-30.	0.6	14
31	Insights into the Phase Relations in a U-N System Using a Cluster Formula. <i>Inorganic Chemistry</i> , 2017, 56, 3550-3555.	1.9	7
32	Stability and optical properties of plutonium monoxide from first-principle calculation. <i>Scientific Reports</i> , 2017, 7, 12167.	1.6	13
33	Electronic structures of topological insulator Bi ₂ Te ₃ surfaces with non-conventional terminations. <i>New Journal of Physics</i> , 2016, 18, 093015.	1.2	13
34	Differences in the Existence States of Hydrogen in UO ₂ and PuO ₂ from DFT + <i>U</i> Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18445-18451.	1.5	34
35	Interfacial properties and electron structure of Al/B ₄ C interface: A first-principles study. <i>Journal of Nuclear Materials</i> , 2016, 478, 227-235.	1.3	63
36	First-principles studies on the charge density wave in uranium. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016, 24, 055011.	0.8	4

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37	First-principles DFT +U calculations on the energetics of Ga in Pu, Pu ₂ O ₃ and PuO ₂ . Computational Materials Science, 2016, 122, 263-271.	1.4	29
38	A theoretical study of hydrogen atoms adsorption and diffusion on PuO ₂ (110) surface. Journal of Alloys and Compounds, 2016, 666, 287-291.	2.8	16
39	New insight into the intrinsic instability of fcc ZrH ₂ by energy-resolved local bonding analysis. RSC Advances, 2016, 6, 19150-19154.	1.7	4
40	Adsorption and dissociation of H ₂ on PuO ₂ (110) surface: A density functional theory study. Journal of Alloys and Compounds, 2016, 654, 567-573.	2.8	16
41	First-Principles Energetics of Some Nonmetallic Impurity Atoms in Plutonium Dioxide. Journal of Physical Chemistry C, 2015, 119, 14879-14889.	1.5	24
42	Novel $\langle \text{mml:math altimg="si1.gif" overflow="scroll"} \rangle$ $\text{xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema"}$ $\text{xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd"}$ $\text{xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML"}$ $\text{xmlns:tb="http://www.elsevier.com/xml/common/table/dtd"}$ $\text{xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd"}$ $\text{xmlns:ce="http://www.elsevier.com/x"}$	0.9	2
43	New Insights into the Formation of Hyperstoichiometric Plutonium Oxides. Journal of Physical Chemistry C, 2015, 119, 101-108.	1.5	26
44	Single-mode approximation for quantum Hall states with broken rotational symmetry. Physical Review B, 2013, 88, .	1.1	5
45	Model anisotropic quantum Hall states. Physical Review B, 2012, 85, .	1.1	69
46	Quantum Hall effects in fast-rotating Fermi gases with anisotropic dipolar interaction. Physical Review A, 2011, 83, .	1.0	25
47	Dynamical properties of a trapped dipolar Fermi gas at finite temperature. Physical Review A, 2011, 83, .	1.0	10
48	Spatial density oscillations in trapped dipolar condensates. Physical Review A, 2010, 82, .	1.0	50