Takuji Oda

List of Publications by Year
in descending order

50 papers	593 citations	687363 13 h-index	642732 23 g-index
50 all docs	50 docs citations	50 times ranked	650 citing authors

#	Article	IF	Citations
1	Correction methods for first-principles calculations of the solution enthalpy of gases and compounds in liquid metals. Physical Chemistry Chemical Physics, 2022, 24, 757-770.	2.8	3
2	First-Principles Calculations of the Diffusivity of Interstitial Helium in Alpha-U Considering Anisotropy, Isotope Effects, and Quantum Effects. Journal of Physical Chemistry C, 2021, 125, 21101-21111.	3.1	3
3	Tritium and helium embrittlement of austenitic steels used in tritium storage and delivery system. Journal of Nuclear Materials, 2020, 540, 152349.	2.7	7
4	Solution enthalpy calculation for impurity in liquid metal by first-principles calculations: A benchmark test for oxygen impurity in liquid sodium. Journal of Chemical Physics, 2020, 152, 154503.	3.0	4
5	Comparison and validation of the lattice thermal conductivity formulas used in equilibrium molecular dynamics simulations for binary systems. Computational Materials Science, 2020, 178, 109615.	3.0	2
6	A comparative study on modeling of the ferromagnetic and paramagnetic states of uranium hydride using a DFT+U method. Physical Chemistry Chemical Physics, 2019, 21, 17628-17639.	2.8	5
7	Characterization and quantification of numerical errors in threshold displacement energy calculated by molecular dynamics in bcc-Fe. Computational Materials Science, 2019, 170, 109189.	3.0	4
8	Chemical origin of differences in steel corrosion behaviors of s-electron and p-electron liquid metals by first-principles calculation. Physical Chemistry Chemical Physics, 2019, 21, 25916-25924.	2.8	1
9	Atomistic simulation for strain effects on threshold displacement energies in refractory metals. Computational Materials Science, 2019, 158, 346-352.	3.0	13
10	Structural and chemical analysis of second-row impurities in liquid leadâ€“bismuth eutectic by first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2018, 20, 30480-30491.	2.8	6
11	Molecular dynamics simulation on stability and diffusivity of hydrogen around a <111> symmetric tilt grain boundary in bcc-Fe. Fusion Engineering and Design, 2018, 131, 105-110.	1.9	6
12	Performance of exchange-correlation functionals in density functional theory calculations for liquid metal: A benchmark test for sodium. Journal of Chemical Physics, 2018, 148, 144501.	3.0	5
13	Chemical states of 3d transition metal impurities in a liquid leadâ€“bismuth eutectic analyzed using first principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 9945-9956.	2.8	16
14	Evaluation of the threshold displacement energy in tungsten by molecular dynamics calculations. Journal of Nuclear Materials, 2017, 495, 277-284.	2.7	33
15	Experiment to Recover Tritium from Li-Pb Blanket and Understanding Chemistry of the Li17Pb83â€“H System. Fusion Science and Technology, 2017, , 1-8.	1.1	2
16	Thermodynamic model for grain boundary effects on hydrogen solubility, diffusivity and permeability in poly-crystalline tungsten. Fusion Engineering and Design, 2016, 112, 102-116.	1.9	26
17	Trap effect of vacancy on hydrogen diffusivity in bcc-Fe. Journal of Nuclear Materials, 2016, 469, 237-243.	2.7	16
18	Two-body potential model based on cosine series expansion for ionic materials. Computational Materials Science, 2016, 111, 54-63.	3.0	1

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19	Kinetic Monte Carlo simulation on influence of vacancy on hydrogen diffusivity in tungsten. Journal of Nuclear Materials, 2015, 467, 439-447.	2.7	35
20	Influence of surface morphology and surface area on release behavior of hydrogen isotopes in LiNbO 3. Fusion Engineering and Design, 2014, 89, 2797-2805.	1.9	1
21	First-principles calculations for the surface termination of Li2TiO3(001) surfaces. Journal of Nuclear Materials, 2013, 442, S705-S709.	2.7	3
22	Optimization of a hybrid exchangeâ€“correlation functional for silicon carbides. Chemical Physics Letters, 2013, 579, 58-63.	2.6	9
23	Deuterium trapping by irradiation damage in tungsten induced by different displacement processes. Fusion Engineering and Design, 2013, 88, 1749-1752.	1.9	27
24	Release behavior of hydrogen isotopes thermally sorbed in Li2TiO3 single crystal. Journal of Nuclear Materials, 2013, 442, S437-S441.	2.7	14
25	Scanning Tunneling Microscopy and Molecular Dynamics Study of the Li₂TiO₃(001) Surface. Journal of Physical Chemistry C, 2013, 117, 5126-5131.	3.1	21
26	Study of intrinsic defects in 3C-SiC using first-principles calculation with a hybrid functional. Journal of Chemical Physics, 2013, 139, 124707.	3.0	27
27	Nanoscale engineering of radiation tolerant silicon carbide. Physical Chemistry Chemical Physics, 2012, 14, 13429.	2.8	98
28	Effect of Grain Size on Hydrogen Isotope Behavior in LiNbO₃. Fusion Science and Technology, 2011, 60, 1147-1150.	1.1	3
29	Development of Tritium Recovery by Flowing O2+Ar Gases at Steam Generator in Fast Breeder Reactor. Fusion Science and Technology, 2011, 60, 1423-1426.	1.1	1
30	Modeling of diffusivity of tritium interacting with F centers in Li2O. Journal of Nuclear Materials, 2011, 417, 743-747.	2.7	4
31	Correlation between surface hydroxyl behavior and surface oxidation state of F82H. Journal of Nuclear Materials, 2011, 417, 1139-1142.	2.7	0
32	Vibration analysis of Oâ€“H stretching mode in Mg(OH)2, Ca(OH)2, LiOH, and NaOH by plane-wave pseudopotential DFT calculation. Computational and Theoretical Chemistry, 2011, 963, 215-220.	2.5	12
33	Comparison of deuterium retention for ion-irradiated and neutron-irradiated tungsten. Physica Scripta, 2011, T145, 014050.	2.5	42
34	Release behavior of hydrogen isotopes thermally absorbed in lithium niobate. Fusion Engineering and Design, 2010, 85, 1772-1776.	1.9	1
35	Modeling of Li diffusivity in Li2O by molecular dynamics simulation. Journal of Nuclear Materials, 2009, 386-388, 1087-1090.	2.7	19
36	Chemical state and diffusion behavior of hydrogen isotopes in liquid lithiumâ€“lead. Chemical Physics Letters, 2009, 483, 214-218.	2.6	13

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37	IR observation on Oâ€“D vibration in LiNbO3 and LiTaO3 single crystal irradiated by 3keV. Journal of Nuclear Materials, 2008, 382, 46-50.	2.7	5
38	Existence states of deuterium irradiated into LiAlO2. Journal of Nuclear Materials, 2008, 372, 53-58.	2.7	11
39	Monte Carlo Simulation on Permeation of Hydrogen Isotopes Through bcc Fe. Fusion Science and Technology, 2008, 54, 537-540.	1.1	6
40	Recovery of Tritium Dissolved in Sodium at the Steam Generator of Fast Breeder Reactor. Fusion Science and Technology, 2008, 54, 337-340.	1.1	1
41	Effects of helium implantation on hydrogen isotope retention behavior in SiC. Journal of Nuclear Materials, 2007, 363-365, 933-937.	2.7	8
42	Validation of potential models for Li2O in classical molecular dynamics simulation. Journal of Nuclear Materials, 2007, 367-370, 263-268.	2.7	19
43	Development of partial-charge potential for GaN. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 50-53.	1.4	4
44	Reactivity of H2O gas with the surface of polycrystalline Li2O pellet. Fusion Engineering and Design, 2006, 81, 613-618.	1.9	5
45	Dynamic observation of the behavior of 3keV irradiated into Li2O using IR absorption spectroscopy. Journal of Nuclear Materials, 2005, 346, 306-311.	2.7	12
46	Behavior of Li2TiO3 under varied surface condition. Fusion Engineering and Design, 2005, 75-79, 765-768.	1.9	9
47	Thermal desorption behavior of hydrogen isotopes interacting with radiation defects in Li2O. Fusion Engineering and Design, 2005, 75-79, 835-839.	1.9	7
48	Hydrogen isotope behavior in Li2O at low temperature by FT-IR. Journal of Nuclear Materials, 2004, 329-333, 1270-1273.	2.7	5
49	Observation of multiple Oâ€“D vibration peaks in Li2O using FT-IR. Journal of Nuclear Materials, 2004, 329-333, 1256-1259.	2.7	6
50	UPS Study on the Interaction of Hydrogen Isotopes with Li₂O Surface. Fusion Science and Technology, 2003, 44, 485-489.	1.1	12