## Dezhou Guo

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Increasing Oxygen Balance Leads to Enhanced Performance in Environmentally Acceptable High-Energy Density Materials: Predictions from First-Principles Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2022, 14, 5257-5264.	4.0	9
2	Chemisorption-Induced Formation of Biphenylene Dimer on Ag(111). Journal of the American Chemical Society, 2022, 144, 723-732.	6.6	20
3	Dislocation-mediated shear amorphization in boron carbide. Science Advances, 2021, 7, .	4.7	49
4	Elucidating the Cooperative Roles of Water and Lewis Acid–Base Pairs in Cascade C–C Coupling and Self-Deoxygenation Reactions. Jacs Au, 2021, 1, 1471-1487.	3.6	5
5	Thermal decomposition and diffusion of methane in clathrate hydrates from quantum mechanics simulations. RSC Advances, 2020, 10, 14753-14760.	1.7	3
6	Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide. Journal of Physical Chemistry C, 2020, 124, 9787-9794.	1.5	10
7	Graphite interface mediated grain-boundary sliding leads to enhanced mechanical properties of nanocrystalline silicon carbide. Materialia, 2019, 7, 100394.	1.3	6
8	Transgranular amorphous shear band formation in polycrystalline boron carbide. International Journal of Plasticity, 2019, 121, 218-226.	4.1	14
9	Thermal Stability and Detonation Properties of Potassium 4,4′-Bis(dinitromethyl)-3,3′-azofurazanate, an Environmentally Friendly Energetic Three-Dimensional Metal–Organic Framework. ACS Applied Materials & Interfaces, 2019, 11, 1512-1519.	4.0	23
10	Grain Boundary Sliding and Amorphization are Responsible for the Reverse Hall-Petch Relation in Superhard Nanocrystalline Boron Carbide. Physical Review Letters, 2018, 121, 145504.	2.9	73
11	Influence of Silicon on the Detonation Performance of Energetic Materials from First-Principles Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 24481-24487.	1.5	9
12	Dual Functions of Water in Stabilizing Metal-Pentazolate Hydrates [M(N <sub>5</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> ]·4H <sub>2</sub> O (M = Mn, Fe, Co,) Tj E	ТФф000	rgBT /Overlo
13	Prediction of the Chapman–Jouguet chemical equilibrium state in a detonation wave from first principles based reactive molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 2015-2022.	1.3	35
14	The co-crystal of TNT/CL-20 leads to decreased sensitivity toward thermal decomposition from first principles based reactive molecular dynamics. Journal of Materials Chemistry A, 2015, 3, 5409-5419.	5.2	89

15Compressive Shear Reactive Molecular Dynamics Studies Indicating That Cocrystals of TNT/CL-201.56515Decrease Sensitivity. Journal of Physical Chemistry C, 2014, 118, 30202-30208.1.565