

Difan Zhang

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Computational Study of Low Interlayer Friction in $Ti_{n+1}C_n$ ($n = 1, 2, \text{ and } 3$) MXene. ACS Applied Materials & Interfaces, 2017, 9, 34467-34479.	8.0	93
2	Multiscale computational understanding and growth of 2D materials: a review. Npj Computational Materials, 2020, 6, .	8.7	89
3	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie - International Edition, 2021, 60, 290-296.	13.8	40
4	Graphene-Titanium Interfaces from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 33288-33297.	8.0	37
5	Molecular Simulation of Capture of Sulfur-Containing Gases by Porous Aromatic Frameworks. Journal of Physical Chemistry C, 2018, 122, 18456-18467.	3.1	31
6	Probing the accuracy of reactive and non-reactive force fields to describe physical and chemical properties of graphene-oxide. Computational Materials Science, 2016, 114, 236-243.	3.0	26
7	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	3.1	25
8	Molecular-Level Overhaul of Aminopropyl Aminosilicone/Triethylene Glycol Post-Combustion CO_2 Capture Solvents. ChemSusChem, 2020, 13, 3429-3438.	6.8	16
9	Computational investigation on CO_2 adsorption in titanium carbide-derived carbons with residual titanium. Carbon, 2017, 111, 741-751.	10.3	14
10	Hydrogen Bonding Enhances the Electrochemical Hydrogenation of Benzaldehyde in the Aqueous Phase. Angewandte Chemie, 2021, 133, 294-300.	2.0	12
11	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. MRS Advances, 2018, 3, 457-462.	0.9	7
12	The structure of graphene on graphene/ C_{60} /Cu interfaces: a molecular dynamics study. Nanotechnology, 2019, 30, 505707.	2.6	7
13	Dynamics of graphene/Al interfaces using COMB3 potentials. Physical Review Materials, 2019, 3, .	2.4	7
14	Tuning the Charge and Hydrophobicity of Graphene Oxide Membranes by Functionalization with Ionic Liquids at Epoxide Sites. ACS Applied Materials & Interfaces, 2022, 14, 19031-19042.	8.0	6
15	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	2.8	3
16	Advanced Theory and Simulation to Guide the Development of CO_2 Capture Solvents. ACS Omega, 2022, 7, 12453-12466.	3.5	2
17	AMPHIPHILIC WATER-LEAN CARBON CAPTURE SOLVENT WETTING BEHAVIOR VIA DECOMPOSITION BY STAINLESS-STEEL INTERFACES. ChemSusChem, 2021, 14, 5283-5292.	6.8	1
18	Computational and Experimental Study for the Denitrification of Biomass-Derived Hydrothermal Liquefaction Oil. ACS Sustainable Chemistry and Engineering, 2021, 9, 13406-13413.	6.7	1