

Nadire Nayir

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

15
papers

136
citations

6
h-index

11
g-index

20
ext. papers

212
ext. citations

5.2
avg, IF

2.8
L-index

#	Paper	IF	Citations
15	Atomic-scale probing of defect-assisted Ga intercalation through graphene using ReaxFF molecular dynamics simulations. <i>Carbon</i> , 2022 , 190, 276-290	10.4	3
14	Density functional study of Ga intercalation at graphene/SiC heterointerface. <i>Journal of Materials Research</i> , 2022 , 37, 1172-1182	2.5	1
13	Understanding physical chemistry of BaSrTiO using ReaxFF molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 25056-25062	3.6	
12	INDEEDopt: a deep learning-based ReaxFF parameterization framework. <i>Npj Computational Materials</i> , 2021 , 7,	10.9	6
11	Development and Applications of ReaxFF Reactive Force Fields for Group-III Gas-Phase Precursors and Surface Reactions with Graphene in MetalOrganic Chemical Vapor Deposition Synthesis. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 10747-10758	3.8	3
10	Illuminating Invisible Grain Boundaries in Coalesced Single-Orientation WS Monolayer Films. <i>Nano Letters</i> , 2021 , 21, 6487-6495	11.5	7
9	A ReaxFF Force Field for 2D-WS ₂ and Its Interaction with Sapphire. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 17950-17961	3.8	3
8	Theoretical modeling of edge-controlled growth kinetics and structural engineering of 2D-MoSe ₂ . <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021 , 271, 115263	3.1	3
7	Modeling for Structural Engineering and Synthesis of Two-Dimensional WSe ₂ Using a Newly Developed ReaxFF Reactive Force Field. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 28285-28297	3.8	10
6	Atomically thin half-van der Waals metals enabled by confinement heteroepitaxy. <i>Nature Materials</i> , 2020 , 19, 637-643	27	53
5	Development of the ReaxFF Reactive Force Field for Inherent Point Defects in the Si/Silica System. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 4303-4313	2.8	10
4	Multi-scale modeling of gas-phase reactions in metal-organic chemical vapor deposition growth of WSe ₂ . <i>Journal of Crystal Growth</i> , 2019 , 527, 125247	1.6	25
3	Development of a ReaxFF Reactive Force Field for Interstitial Oxygen in Germanium and Its Application to GeO ₂ /Ge Interfaces. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 1208-1218	3.8	8
2	Structural properties of indium phosphide nanorods: molecular dynamics simulations. <i>International Journal of Nanotechnology</i> , 2016 , 13, 809	1.5	
1	An Initial Design-enhanced Deep Learning-based Optimization Framework to Parameterize Multicomponent ReaxFF Force Fields		3