Menno Bokdam

List of Publications by Year in Descending Order

20 papers	1,164 citations	16 h-index	22 g-index
22 ext. papers	1,374 ext. citations	5.1 avg, IF	4.5 L-index

#	Paper	IF	Citations
20	Microscopic (Dis)order and Dynamics of Cations in Mixed FA/MA Lead Halide Perovskites. *Journal of Physical Chemistry C*, **2021**, 125, 1742-1753	3.8	14
19	Exploring Librational Pathways with on-the-Fly Machine-Learning Force Fields: Methylammonium Molecules in MAPbX (X = I, Br, Cl) Perovskites. *Journal of Physical Chemistry C*, **2021**, 125, 21077-21086	3.8	1
18	Long-range order imposed by short-range interactions in methylammonium lead iodide: Comparing point-dipole models to machine-learning force fields. *Physical Review B*, **2019**, 100,	3.3	9
17	Phase Transitions of Hybrid Perovskites Simulated by Machine-Learning Force Fields Trained on the Fly with Bayesian Inference. *Physical Review Letters*, **2019**, 122, 225701	7.4	106
16	Finite-temperature structure of the MAPbI3 perovskite: Comparing density functional approximations and force fields to experiment. *Physical Review Materials*, **2018**, 2,	3.2	21
15	Assessing Density Functionals Using Many Body Theory for Hybrid Perovskites. *Physical Review Letters*, **2017**, 119, 145501	7.4	43
14	Dipole Order in Halide Perovskites: Polarization and Rashba Band Splittings. *Journal of Physical Chemistry C*, **2017**, 121, 23045-23054	3.8	39
13	Behavior of Methylammonium Dipoles in MAPbX (X = Br and I). *Journal of Physical Chemistry Letters*, **2017**, 8, 4113-4121	6.4	76
12	Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites. *Scientific Reports*, **2016**, 6, 28618	4.9	178
11	Z_{2} Invariance of Germanene on MoS_{2} from First Principles. *Physical Review Letters*, **2016**, 116, 256805	7.4	29
10	Room-temperature dynamic correlation between methylammonium molecules in lead-iodine based perovskites: An ab initio molecular dynamics perspective. *Physical Review B*, **2016**, 94,	3.3	51
9	Band gaps in incommensurable graphene on hexagonal boron nitride. *Physical Review B*, **2014**, 89,	3.3	81
8	Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites. *Nature Communications*, **2014**, 5, 5900	17.4	215
7	Schottky barriers at hexagonal boron nitride/metal interfaces: A first-principles study. *Physical Review B*, **2014**, 90,	3.3	62
6	Large potential steps at weakly interacting metal-insulator interfaces. *Physical Review B*, **2014**, 90,	3.3	16
5	Field effect doping of graphene in metal|dielectric|graphene heterostructures: A model based upon first-principles calculations. *Physical Review B*, **2013**, 87,	3.3	30
4	Modeling charge transfer at organic donor-acceptor semiconductor interfaces. *Applied Physics Letters*, **2012**, 100, 203302	3.4	25

3	Charge equilibration and potential steps in organic semiconductor multilayers. *Organic Electronics*, **2012**, 13, 1793-1801	3.5	19
2	Electrostatic doping of graphene through ultrathin hexagonal boron nitride films. *Nano Letters*, **2011**, 11, 4631-5	11.5	107
1	Fermi level pinning by integer charge transfer at electrode-organic semiconductor interfaces. *Applied Physics Letters*, **2011**, 98, 113303	3.4	41