## Jaebeom Han

List of Publications by Year in descending order

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LAEREOM HAN

#	Article	IF	CITATIONS
1	Determining the atomic charge of calcium ion requires the information of its coordination geometry in an EF-hand motif. Journal of Chemical Physics, 2021, 154, 124104.	3.0	6
2	On the Interplay between Electronic Structure and Polarizable Force Fields When Calculating Solution-Phase Charge-Transfer Rates. Journal of Chemical Theory and Computation, 2020, 16, 6481-6490.	5.3	6
3	Calculated Reduction Potentials of Electrolyte Species in Lithium–Sulfur Batteries. Journal of Physical Chemistry C, 2020, 124, 20654-20670.	3.1	18
4	First-principles calculations of oxidation potentials of electrolytes in lithium–sulfur batteries and their variations with changes in environment. Physical Chemistry Chemical Physics, 2018, 20, 18811-18827.	2.8	8
5	Quantum mechanical force field for water with explicit electronic polarization. Journal of Chemical Physics, 2013, 139, 054503.	3.0	36
6	Optimization of the explicit polarization (X-Pol) potential using a hybrid density functional. Theoretical Chemistry Accounts, 2012, 131, 1161.	1.4	15
7	Explicit Polarization (X-Pol) Potential Using ab Initio Molecular Orbital Theory and Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 11656-11664.	2.5	49
8	Nitrile and thiocyanate IR probes: Molecular dynamics simulation studies. Journal of Chemical Physics, 2008, 128, 154504.	3.0	124
9	Site-Specific Hydrogen-Bonding Interaction between N-Acetylproline Amide and Protic Solvent Molecules:  Comparisons of IR and VCD Measurements with MD Simulations. Journal of Physical Chemistry A, 2006, 110, 13355-13365.	2.5	20
10	Phenol-benzene complexation dynamics: Quantum chemistry calculation, molecular dynamics simulations, and two dimensional IR spectroscopy. Journal of Chemical Physics, 2006, 125, 244508.	3.0	49
11	Temperature-dependent growth of carbon nanotubes by pyrolysis of ferrocene and acetylene in the range between 700 and 1000 °C. Chemical Physics Letters, 2003, 372, 853-859.	2.6	122
12	Vertically Aligned Carbon Nanotubes Grown by Pyrolysis of Iron, Cobalt, and Nickel Phthalocyanines. Journal of Physical Chemistry B, 2003, 107, 9249-9255.	2.6	133