

# Daniela Kohen

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Atomistic Simulations of CO <sub>2</sub> and N <sub>2</sub> Adsorption in Silica Zeolites: The Impact of Pore Size and Shape. Journal of Physical Chemistry B, 2002, 106, 8367-8375.	2.6	205
2	Model studies of nonadiabatic dynamics. Journal of Chemical Physics, 1998, 109, 4713-4725.	3.0	84
3	Computational Chemistry Methods for Nanoporous Materials. Chemistry of Materials, 2017, 29, 199-212.	6.7	69
4	Molecular Insight into CO <sub>2</sub> "Trapdoor" Adsorption in Zeolite Na-RHO. Chemistry of Materials, 2017, 29, 2724-2730.	6.7	64
5	Simulation of nonadiabatic wave packet interferometry using classical trajectories. Journal of Chemical Physics, 2000, 112, 7345-7354.	3.0	60
6	Phase space distribution function formulation of the method of reactive flux: Memory friction. Journal of Chemical Physics, 1995, 103, 6013-6020.	3.0	49
7	Derivation of Kramers' formula for condensed phase reaction rates using the method of reactive flux. Journal of Chemical Physics, 1994, 100, 4932-4940.	3.0	37
8	Modeling the interaction of hydrogen with silicon surfaces. Surface Science, 1998, 397, 225-236.	1.9	30
9	Atomistic Simulations of CO <sub>2</sub> and N <sub>2</sub> Diffusion in Silica Zeolites: The Impact of Pore Size and Shape. Journal of Physical Chemistry C, 2008, 112, 16521-16531.	3.1	28
10	Quantum adiabatic switching. Journal of Chemical Physics, 1993, 98, 3168-3178.	3.0	24
11	Bimetallic, Silylene-Mediated Multielectron Reductions of Carbon Dioxide and Ethylene. Angewandte Chemie - International Edition, 2021, 60, 1615-1619.	13.8	15
12	Atomistic Simulations of CO <sub>2</sub> and N <sub>2</sub> within Cage-Type Silica Zeolites. Langmuir, 2011, 27, 1954-1963.	3.5	14
13	A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. Fluid Phase Equilibria, 2014, 366, 146-151.	2.5	14
14	A Theoretical Mechanistic Study of the Asymmetric Desymmetrization of a Cyclic meso-Anhydride by a Bifunctional Quinine Sulfonamide Organocatalyst. Journal of Organic Chemistry, 2017, 82, 1347-1355.	3.2	13
15	Nanoscale shock wave spectroscopy: A direct view of coherent ultrafast bath dynamics. Journal of Chemical Physics, 1999, 111, 4343-4350.	3.0	6
16	Bimetallic, Silylene-Mediated Multielectron Reductions of Carbon Dioxide and Ethylene. Angewandte Chemie, 2021, 133, 1639-1643.	2.0	5
17	Cobalt Silylenes as Platforms for Catalytic Nitrene-Group Transfer by Metal-Ligand Cooperation. Angewandte Chemie - International Edition, 2022, , .	13.8	1
18	Cobalt Silylenes as Platforms for Catalytic Nitrene-Group Transfer by Metal-Ligand Cooperation. Angewandte Chemie, 0, , .	2.0	0