## Kulbir K Ghuman

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Role of surface engineering of hybrid structure for high performance quantum dots based photoelectrochemical hydrogen generation. Chemical Engineering Journal, 2022, 429, 132425.	12.7	14
2	Molecular dynamics study of oxygen-ion diffusion in yttria-stabilized zirconia grain boundaries. Journal of Materials Chemistry A, 2022, 10, 2567-2579.	10.3	11
3	Disorder in energy materials and strategies to model it. Advances in Physics: X, 2021, 6, .	4.1	1
4	Shining light on CO <sub>2</sub> : from materials discovery to photocatalyst, photoreactor and process engineering. Chemical Society Reviews, 2020, 49, 5648-5663.	38.1	91
5	Microstructural and Electronic Properties of the YSZ/CeO <sub>2</sub> Interface via Multiscale Modeling. Journal of Physical Chemistry C, 2020, 124, 15680-15687.	3.1	2
6	Interfacial Properties of Bilayer SOFC Electrolytes Via Scale Bridging Simulations. ECS Meeting Abstracts, 2020, MA2020-01, 1801-1801.	0.0	0
7	Tailoring widely used ammonia synthesis catalysts for H and N poisoning resistance. Physical Chemistry Chemical Physics, 2019, 21, 5117-5122.	2.8	13
8	Mechanistic insights into water adsorption and dissociation on amorphous TiO <sub>2</sub> -based catalysts. Science and Technology of Advanced Materials, 2018, 19, 44-52.	6.1	25
9	Highly Efficient Ambient Temperature CO <sub>2</sub> Photomethanation Catalyzed by Nanostructured RuO <sub>2</sub> on Silicon Photonic Crystal Support. Advanced Energy Materials, 2018, 8, 1702277.	19.5	58
10	Solar Fuels: Highly Efficient Ambient Temperature CO <sub>2</sub> Photomethanation Catalyzed by Nanostructured RuO <sub>2</sub> on Silicon Photonic Crystal Support (Adv. Energy Mater. 9/2018). Advanced Energy Materials, 2018, 8, 1870041.	19.5	7
11	Tailoring Surface Frustrated Lewis Pairs of In <sub>2</sub> O <sub>3â^'</sub> <i><sub>x</sub></i> (OH) <sub>y</sub> for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO <sub>2</sub> by Isomorphous Substitution of In <sup>3+</sup> with Bi <sup>3+</sup> . Advanced Science, 2018, 5, 1700732.	11.2	91
12	Enhanced photothermal reduction of gaseous CO <sub>2</sub> over silicon photonic crystal supported ruthenium at ambient temperature. Energy and Environmental Science, 2018, 11, 3443-3451.	30.8	83
13	Solar Fuels: Tailoring Surface Frustrated Lewis Pairs of In <sub>2</sub> O <sub>3â<sup>~</sup></sub> <i><sub>x</sub></i> (OH) <sub>y</sub> for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO <sub>2</sub> by Isomorphous Substitution of In <sup>3+</sup> with Bi <sup>3+</sup> (Adv. Sci. 6/2018) Advanced Science, 2018, 5, 1870034	11.2	3
14	Electronic Structure of a Polybenzimidazole-Wrapped Single-Wall Carbon Nanotube. Journal of Physical Chemistry C, 2018, 122, 15979-15985.	3.1	7
15	Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO <sub>2</sub> with High Activity and Tailored Selectivity. Advanced Science, 2017, 4, 1700252.	11.2	97
16	Photothermal Catalysis: Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO <sub>2</sub> with High Activity and Tailored Selectivity (Adv. Sci. 10/2017). Advanced Science, 2017, 4, .	11.2	2
17	Self-Trapped Charge Carriers in Defected Amorphous TiO <sub>2</sub> . Journal of Physical Chemistry C, 2016, 120, 27910-27916.	3.1	17
18	Carrier dynamics and the role of surface defects: Designing a photocatalyst for gas-phase CO <sub>2</sub> reduction. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8011-E8020.	7.1	89

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19	Surface Analogues of Molecular Frustrated Lewis Pairs in Heterogeneous CO <sub>2</sub> Hydrogenation Catalysis. ACS Catalysis, 2016, 6, 5764-5770.	11.2	80
20	Metadynamics-Biased ab Initio Molecular Dynamics Study of Heterogeneous CO <sub>2</sub> Reduction via Surface Frustrated Lewis Pairs. ACS Catalysis, 2016, 6, 7109-7117.	11.2	78
21	Heterogeneous reduction of carbon dioxide by hydride-terminated silicon nanocrystals. Nature Communications, 2016, 7, 12553.	12.8	93
22	Photoexcited Surface Frustrated Lewis Pairs for Heterogeneous Photocatalytic CO <sub>2</sub> Reduction. Journal of the American Chemical Society, 2016, 138, 1206-1214.	13.7	210
23	Illuminating CO <sub>2</sub> reduction on frustrated Lewis pair surfaces: investigating the role of surface hydroxides and oxygen vacancies on nanocrystalline In <sub>2</sub> O <sub>3â<sup>^</sup>x</sub> (OH) <sub>y</sub> . Physical Chemistry Chemical Physics, 2015, 17, 14623-14635.	2.8	186
24	Adsorption and Dissociation of H <sub>2</sub> O on Monolayered MoS <sub>2</sub> Edges: Energetics and Mechanism from <i>ab Initio</i> Simulations. Journal of Physical Chemistry C, 2015, 119, 6518-6529.	3.1	107
25	A DFT + <i>U</i> study of (Rh, Nb)-codoped rutile TiO <sub>2</sub> . Journal of Physics Condensed Matter, 2013, 25, 085501.	1.8	23
26	Vibrational density of states of TiO2 nanoparticles. Journal of Non-Crystalline Solids, 2013, 373-374, 28-33.	3.1	6
27	Effect of doping on electronic structure and photocatalytic behavior of amorphous TiO2. Journal of Physics Condensed Matter, 2013, 25, 475501.	1.8	30
28	Amorphous TiO2 as a Photocatalyst for Hydrogen Production: A DFT Study of Structural and Electronic Properties. Energy Procedia, 2012, 29, 291-299.	1.8	108
29	Structural properties of amorphous TiO2 nanoparticle: Molecular dynamics study. , 2011, , .		0
30	Structure factor of amorphous TiO2 nanoparticle; Molecular Dynamics Study. Journal of Non-Crystalline Solids, 2011, 357, 3399-3404.	3.1	19
31	Meyer–Neldel DC conduction in chalcogenide glasses. Pramana - Journal of Physics, 2011, 76, 629-637.	1.8	6
32	Strained structure of differently prepared amorphous TiO <sub>2</sub> nanoparticle: Molecular dynamics study. Journal of Materials Research, 2011, 26, 2604-2611.	2.6	14
33	Static Structure Factor of Amorphous Rutile Nanoparticle: A Molecular Dynamics Study. , 2011, , .		0