Consiglio Nazionale delle Ricerche

Istituto di Chimica e della Materia Condensata e di Tecnologie per l'Energia

ICMATE

From PEGylated ZnO Nanostructures to Electrocatalytic Hybrid Proton Exchange Membranes: A Systematic Approach for Sustainable Hydrogen Production

Abstract:

The rational design of multifunctional materials for hydrogen energy requires a unified strategy that connects nanoscale synthesis, bandgap engineering, and device-level performance. We first investigated the polyethylene glycol (PEG)-assisted hydrothermal synthesis of ZnO nanoparticles using PEG molecular weights of 8000, 10000, and 20000. Among these, the PEG 20k-assisted sample exhibited the most uniform spherical morphology (≈ 40 nm), the lowest bandgap (3.02 eV), and superior electrochemical performance, delivering a current density of 267.83 mA cm^{-2} under acidic conditions with a Volmer-step-limited hydrogen evolution reaction (HER, Tafel slope 147 mV dec^{-1}). Building on this, we explored bandgap tuning of transition metal oxides (Co_3O_4, CuO, ZnO) via PEGylation, showing that solvation energy-driven lattice parameter modulation enables significant bandgap alteration independent of size confinement. ZnO displayed the maximum tunability (7.33%), strongly correlated with orientation-dependent lattice distortions, providing a fundamental framework for solvation-assisted band engineering. Finally, these insights were applied to fabricate a ZnO-incorporated hybrid catalytic proton exchange membrane (PEM) by embedding pegylated ZnO into a (diethyl methylamine)/($H_2PO_4^-$) matrix. The resulting p-type MOF-based PEM exhibited a bandgap of 3.67 eV, high proton conductivity (0.027 S cm^{-1} at 300 K, $t^+ > 0.99$), excellent catalytic activity (Tafel slope ~36 mV dec^{-1}), and long-term stability (168 h at pH 7), achieving a current density of 1.52 mA cm^{-2}

Bioskecth:

Prof. Prabhakar Singh holds a Ph.D. from the University of Muenster, Germany. He is currently serving as a Professor of Physics at the Indian Institute of Technology (IIT), Banaras Hindu University (BHU), Varanasi, and occupies the prestigious position of Professor on the HAG Scale. Prof. Singh completed his M.Sc. in Physics and M.Tech. in Materials Science and Technology from Banaras Hindu University (BHU), Varanasi. He earned his B.Sc. degree from Udai Pratap College, Varanasi. With over two decades of academic and research experience, Prof. Singh has made significant contributions to his field. He has published more than 170 peer-reviewed international research papers, authored 14 book chapters, and written a monograph. Additionally, he is one of the editors of the book *Nanomaterials: Advances and Applications*. His research interests span the physics of materials for energy applications, including solid oxide fuel cells, solar cells, and piezoelectric/dielectric materials. Prof. Singh has guided 17 Ph.D. students and 18 Master's students and has mentored several postdoctoral researchers under various national fellowship schemes. As an active collaborator in the global academic community, Prof. Singh has visited several countries to pursue research and foster international collaborations. He is a member of numerous national and international professional societies and has participated in over 80 national and international conferences, delivering invited talks at many of these events. His scholarly contributions have earned him multiple awards and fellowships, including the *Global Star Award (2021)* and *ACerS Global Ambassador awards (2023)* by the American Ceramic Society; and *OVDF-Fellowship* by ANRF, India.

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Seminar "MATERIALS MATTER!"

Invited Speaker: **Prof. Prabhakar Singh**
Department of Physics - BHU
Indian Institute of Technology
Varanasi- India

Date: December 1st, 3.00 pm

Place: UNIGE - Villa Cambiaso, 6 - Auditorium

Participation LINK