Code Developments

Moritz Leucke

- Add experimental feature for GW: Global RI with local metric and new integration for 3-center Integrals MR!1968

New Papers involving FHI-aims

Disclaimer: We compile this list by identifying recent publications that cite the 2009 FHI-aims paper (DOI: 10.1016/j.cpc.2009.06.022). Before including any publication, we verify that FHI-aims was used in some capacity within the article. If we have overlooked any published work involving FHI-aims, we apologize for the oversight and welcome you to inform us. This list is intended for informational purposes only.

- "First-principles data-driven approach for assessment of stability of Tc-C systems," R.A. Zaripov, R.A. Eremin, I.S. Humonen, A.V. Krautsou, V.V. Kuznetsov, K.E. German, S.A. Budennyy, and S.V. Levchenko, Acta Materialia 303, 121704 (2026), DOI: 10.1016/j.actamat.2025.121704.

- "The influence of electron transport at perovskite/carbon interfaces to tailor photosupercapacitor devices: A DFT approach," Á.G. Coronel, C. Delesma, C.A. Celaya, and J. Muñiz, Solar Energy 303, 114099 (2026), DOI: 10.1016/j.solener.2025.114099.

- "Understanding pseudocapacitance and the SO 3 2 − reduction mechanism on Fe 3 O 4 electrode surface: A combined theoretical and experimental study," M. Montañez-Molina, C.A. Celaya, O. Castro-Ocampo, D. Frausto, C. Delesma, M. Solórzano, R.L. Porto, J.A.L. Medina, J. Muñiz, and A.K. Cuentas-Gallegos, Electrochimica Acta 543, 147506 (2025), DOI: 10.1016/j.electacta.2025.147506.

- "Optoelectronic and Excitonic Study of XI_2 (X = Si, Ge, Sn, and Pb) Monolayers Envisaging Potential Technological Applications," B.D. Aparicio-Huacarpuma, J.A.D.S. Laranjeira, K.A. Lopes Lima, E.A. Moujaes, A.M.A. Silva, J. Ricardo Sambrano, A. Cavalheiro Dias, and L.A. Ribeiro Júnior, ACS Omega, in print (2025), DOI: 10.1021/acsomega.5c08479.

- "High-throughput computational screening of two-dimensional oxides for high-performance electronic and optoelectronic devices," Z. Yang, X. Yang, Q. Li, Q. Li, J. Dong, Y. Li, L.K. Ang, Y.S. Ang, S. Fang,

and J. Lu, Phys. Rev. Applied 24(5), 054075 (2025), DOI: 10.1103/krhd-vz9q.

- "Defect-driven switchable polarization in SrTiO 3," W. Aggoune, and M. Scheffler, Phys. Rev. Materials 9(11), 114601 (2025), DOI: 10.1103/7sd9-6gll.

- "Bottom-Up Fabrication of Graphene Nanoribbons with Nonalternant 5/7/5 Ring Motifs," Z. Chen, J. Huang, Q. Chen, Y. Wu, X. Chen, D. Han, W. Yang, H. Ding, J. Hu, Q. Xu, C. Wu, Q. Fan, P. Jelínek, and J. Zhu, J. Am. Chem. Soc., jacs.5c13211 (2025), DOI: 10.1021/jacs.5c13211.

- "Interplay of Manganese Doping in Lead-Free Cs_3 Bi_2 Br_9 Nanocrystals," J.H. Martin, E. Ruiz, L. Lezama, S. Ahmad, and S. Kazim, ACS Appl. Opt. Mater. 3(11), 2725–2735 (2025), DOI: 10.1021/acsaom.5c00416.

- "Improving the First-Principles Description of van der Waals Interactions in Bulk Metals," A. Ambrosetti, G.-X. Zhang, L. Jia, H. Sun, C. Chen, P.L. Silvestrelli, and W. Liu, J. Phys. Chem. C 129(47), 21292–21298 (2025), DOI: 10.1021/acs.jpcc.5c06810.

- "Many-Body Description of van der Waals Torque in Two-Dimensional Materials," Z. Kou, Y. Zhou, Z. Jiang, Z. Zhang, A. Tkatchenko, and X. Liu, ACS Nano 19(46), 39783–39792 (2025), DOI: 10.1021/acsnano.5c12390.

- "Ion-Specific Storage and Diffusion Mechanisms in Cross-Linked Layered Phosphorus Electrodes: From Clustering to Correlated Dynamics," V.S. Thakur, and S. Banerjee, J. Phys. Chem. C 129(48), 21355–21363 (2025), DOI: 10.1021/acs.jpcc.5c06846.

- "Molecular Detection Sensitivity at the Sub-Atto-Molar Limit Using Plasmonic Perovskite Nanoplates," S. Samanta, S. Paul, E. Bora, T. Gaur, N. Guchhait, S. Gómez-Graña, D. Sarker, and T. Debnath, ACS Appl. Nano Mater. 8(46), 22389–22399 (2025), DOI: 10.1021/acsanm.5c04272.

- "Monosaccharide Binding to Synthetic Carbohydrate Receptor Microarrays," M.A. Shlain, K. Erzoah Ndede, K. Thakur, A.J. Russo, S. Pasari, I. Nihal, K.L. Matos, Y.S. Zholdassov, M. Marianski, and A.B. Braunschweig, J. Phys. Chem. C 129(46), 20797–20808 (2025), DOI: 10.1021/acs.jpcc.5c06186.

- "Elucidating the Role of NaCl in the on-Surface Synthesis of Conjugated Azaacene Polymers on Au(111)," T. Kratky, X. Liu, S. Günther, P. Mutombo, L. Schio, L. Floreano, S. Decurtins, J. Repp, P.

Jelínek, S. Liu, and L.L. Patera, Chemistry A European J, e02452 (2025), DOI: 10.1002/chem.202502452.

- "Phosphates and Phosphorylated Amino Acids for the AMOEBA-HFC Polarizable Force Field," J.M. Delgado, G. Schillaci, and S. Varma, J. Chem. Theory Comput. 21(22), 11645–11656 (2025), DOI: 10.1021/acs.jctc.5c01294.

- "Reactivity of an aza-dipyrrin and an aza-BODIPY motif bearing two 2-pyridyl units: an emissive NNN binding pocket," R.L. Gapare, R.M. Diaz-Rodriguez, V.A. Williams, M. Atwood, M.J. Cotnam, J.W. Hilborn, E.R. Johnson, K.N. Robertson, and A. Thompson, Org. Biomol. Chem. 23(45), 10391–10397 (2025), DOI: 10.1039/D5OB01628B.

- "Transforming Bicarbonate to Oxalic Acid: A Photocatalytic Pathway Unveiled by Experiment and Theory," O. Castro-Ocampo, H. Olvera-Vargas, I. Hernández-Pérez, L. González-Reyes, V. Garibay-Febles, J. Muñiz, and R. Suárez-Parra, Top Catal, (2025), DOI: 10.1007/s11244-025-02230-9.

- "Symmetry-Breaking in Carbon Nanohoops Enables Room-Temperature Ternary Single-Molecule Switching," K. Chang, Q. Deng, K. Song, J. Yang, C. Jing, B. Liu, X. Song, Y. Tan, D. Zhu, and Y. Zang, Angewandte Chemie, e19695 (2025), DOI: 10.1002/ange.202519695.

- "A Cu-Based Near-IR Active MOF with an Ion-Pair Guest Exhibiting Versatile and Selective Gas-Solid Reactivity," R. Saha, A. Cortés-Villena, S. Gómez-Coca, A. Fernández-Alarcón, J. Calbo, R.E. Galian, E. Ortí, E. Ruiz, M. Giménez-Marqués, S. Benmansour, and C.J. Gómez-García, Advanced Materials, e13485 (2025), DOI: 10.1002/adma.202513485.

- "Electronic Structure and Interfacial Hole Transfer in a Di-Rhodium Photocatalyst on a p-Type NiO Electrode," F. Fasulo, A. Pecoraro, A.B. Muñoz-García, and M. Pavone, J. Phys. Chem. C 129(44), 20025–20034 (2025), DOI: 10.1021/acs.jpcc.5c05879.

- "An Electrochemical Sensor Based on Polypyrrole and Gold Nanoparticles for Sensitive Detection of 4-Nitrophenol: Experimental and DFT Insights," I. Jasper, A.L. Soares, B.M. Hryniewicz, G.R. Da Silva, S. Weheabby, D. Guedes-Sobrinho, F.L.F. Soares, O. Kanoun, and M. Vidotti, ACS Electrochem. 1(11), 2553–2566 (2025), DOI: 10.1021/acselectrochem.5c00305.

- "Curvature-Directed Selective C–C Bond Cleavage Driven by Electric Fields," X. Song, J.-N. Gao, K. Song, H. Xu, C. Jing, B. Liu, J. Lin, Y. Wang, H. Cong, D. Zhu, and Y. Zang, J. Am. Chem. Soc. 147(44), 40825–40832

(2025), DOI: 10.1021/jacs.5c13861.

- "dpdata: A Scalable Python Toolkit for Atomistic Machine Learning Data Sets," J. Zeng, X. Peng, Y.-B. Zhuang, H. Wang, F. Yuan, D. Zhang, R. Liu, Y. Wang, P. Tuo, Y. Zhang, Y. Chen, Y. Li, C.T. Nguyen, J. Huang, A. Peng, M. Rynik, W.-H. Xu, Z. Zhang, X.-Y. Zhou, T. Chen, J. Fan, W. Jiang, B. Li, D. Li, H. Li, W. Liang, R. Liao, L. Liu, C. Luo, L. Ward, K. Wan, J. Wang, P. Xiang, C. Zhang, J. Zhang, R. Zhou, J.-X. Zhu, L. Zhang, and H. Wang, J. Chem. Inf. Model. 65(21), 11497–11504 (2025), DOI: 10.1021/acs.jcim.5c01767.

- "Polar Triptycene-Based Nonmetal Organic Frameworks Show Enhanced Hydrogen Adsorption," M. O'Shaughnessy, H. Qu, X. Wang, J.B. Holmes, L. Emsley, J. Glover, R. Hafizi, G.M. Day, and A.I. Cooper, J. Am. Chem. Soc. 147(43), 39351–39358 (2025), DOI: 10.1021/jacs.5c11317.

- "The π-Metal-π Motif: A Versatile Design Principle for Rotational Molecular Machines," W. Li, Z. Pan, X. Tan, Y.P. Sarwono, M. Wang, and R. Zhao, J. Phys. Chem. A 129(42), 9840–9850 (2025), DOI: 10.1021/acs.jpca.5c05871.

- "Correct quantification of oxygen vacancies in ferroelectric hafnia," L. Pérez Ramírez, T. Iung, V. Yadav, C. Lubin, U. Schroeder, F. Wunderwald, L. Azevedo Antunes, A. Kersch, T.C. Back, C. Weiland, M. Gros-Jean, and N. Barrett, Journal of Applied Physics 138(13), 134106 (2025), DOI: 10.1063/5.0288354.

Upcoming Events

- Save the date: New FHI-aims webinar on February 25 and 26, 2026 on "Multiscale Modeling with Explicit Embedding Approaches in FHI-aims" with talks by Andrew Logsdail and Gabriel Bramley. More details will follow in the new year!

- Next FHI-aims monthly meeting: THURSDAY, Dec 18, 2025 08:30 AM Eastern Standard Time, US and Canada — More details are posted in the Community Slack Channel!