Stanford



Tom Linker

Casual - Non-Exempt, LCLS - Linac Coherent Light Source

Curriculum Vitae available Online

Bio

BIO

I am an Associate Scientist at SLAC National Lab. I utilize mutliscale simulations and machine learning to understand light matter interaction for ultrafast X-ray experiments performed at X-ray light sources around the world.

I am currently interested in development of attosecond non-linear x-ray emission spectroscopy techniques with the ultimate goal of exploring photochemistry in biological and catalytic systems. I am also developing molecular dynamics frameworks and X-ray scattering/spectroscopy experiments for excited state chemistry at nanoparticle surfaces for new energy technologies.

Publications

PUBLICATIONS

- **Catalysis in Extreme Field Environments: A Case Study of Strongly Ionized SiO2Nanoparticle Surfaces.** *Journal of the American Chemical Society*
  Linker, T. M., Dagar, R., Feinberg, A., Sahel-Schackis, S., Nomura, K., Nakano, A., Shimojo, F., Vashishta, P., Bergmann, U., Kling, M. F., Summers, A. M.
  2024

- **Neutron scattering and neural-network quantum molecular dynamics investigation of the vibrations of ammonia along the solid-to-liquid transition.** *Nature communications*
  Linker, T. M., Krishnamoorthy, A., Daemen, L. L., Ramirez-Cuesta, A. J., Nomura, K., Nakano, A., Cheng, Y. Q., Hicks, W. R., Kolesnikov, A. I., Vashishta, P. D.
  2024; 15 (1): 3911

- **Exploring far-from-equilibrium ultrafast polarization control in ferroelectric oxides with excited-state neural network quantum molecular dynamics.** *Science advances*
  Linker, T., Nomura, K. I., Aditya, A., Fukshima, S., Kalia, R. K., Krishnamoorthy, A., Nakano, A., Rajak, P., Shimmura, K., Shimojo, F., Vashishta, P.
  2022; 8 (12): eabk2625

- **Simultaneous Observation of Carrier-Specific Redistribution and Coherent Lattice Dynamics in 2H-MoTe2 with Femtosecond Core-Level Spectroscopy.** *ACS nano*
  Attar, A. R., Chang, H., Britz, A., Zhang, X., Lin, M., Krishnamoorthy, A., Linker, T., Fritz, D., Neumark, D. M., Kalia, R. K., Nakano, A., Ajayan, P., Vashishta, et al
  2020

- **Ultrahigh energy density in high-temperature polymer dielectric reinforced by bilayer nanocoating** *CHEMICAL ENGINEERING JOURNAL*
  Wang, Y., Linker, T., Lizu, K., Ortiz-Flores, L. A., Kamal, D., Zhou, J., Nguyen, H., Li, C., Gao, W., Konstantinou, A., Chen, L., Huey, B. D., Ramprasad, et al
  2025; 507

- **Tracking surface charge dynamics on single nanoparticles.** *Science advances*
  Dagar, R., Zhang, W., Rosenberger, P., Linker, T. M., Sousa-Castillo, A., Neuhaus, M., Mitra, S., Biswas, S., Feinberg, A., Summers, A. M., Nakano, A., Vashishta, P., Shimojo, et al
  2024; 10 (32): eadp1890

- **Tailoring the Angular Mismatch in MoS2 Homobilayers through Deformation Fields.** *Small (Weinheim an der Bergstrasse, Germany)*
  Burns, K., Tan, A. M., Hachtel, J. A., Aditya, A., Baradwaj, N., Mishra, A., Linker, T., Nakano, A., Kalia, R., Lang, E. J., Schoell, R., Hennig, R. G., Hattar, et al
  2023; 19 (29): e2300098

- **Allegro-Legato: Scalable, Fast, and Robust Neural-Network Quantum Molecular Dynamics via Sharpness-Aware Minimization**
  Ibayashi, H., Razakh, T., Yang, L., Linker, T., Olguin, M., Hattori, S., Luo, Y., Kalia, R. K., Nakano, A., Nomura, K., Vashishta, P.
  edited by Bhatele, A., Hammond, J., Baboulin, M., Kruse, C.
  SPRINGER INTERNATIONAL PUBLISHING AG.2023: 223-239

- **Squishing Skyrmions: Symmetry-Guided Dynamic Transformation of Polar Topologies Under Compression.** *The journal of physical chemistry letters*
  Linker, T., Nomura, K. I., Fukushima, S., Kalia, R. K., Krishnamoorthy, A., Nakano, A., Shimamura, K., Shimojo, F., Vashishta, P.
  2022; 13 (48): 11335-11345

- **Probing the presence and absence of metal-fullerene electron transfer reactions in helium nanodroplets by deflection measurements.** *Physical chemistry chemical physics : PCCP*
  Niman, J. W., Kamerin, B. S., Villers, T. H., Linker, T. M., Nakano, A., Kresin, V. V.
  2022; 24 (17): 10378-10383

- **Deep Well Trapping of Hot Carriers in a Hexagonal Boron Nitride Coating of Polymer Dielectrics.** *ACS applied materials & interfaces*
  Linker, T., Wang, Y., Mishra, A., Kamal, D., Cao, Y., Kalia, R. K., Nakano, A., Ramprasad, R., Shimojo, F., Sotzing, G., Vashishta, P.
  2021; 13 (50): 60393-60400

- **MISTIQS: An open-source software for performing quantum dynamics simulations on quantum computers** *SOFTWAREX*
  Powers, C., Bassman, L., Linker, T. M., Nomura, K., Gulania, S., Kalia, R. K., Nakano, A., Vashishta, P.
  2021; 14

- **Ex-NNQMD: Extreme-Scale Neural Network Quantum Molecular Dynamics**
  Rajak, P., Aditya, A., Fukushima, S., Kalia, R. K., Linker, T., Liu, K., Luo, Y., Nakano, A., Nomura, K., Shimamura, K., Shimojo, F., Vashishta, P., IEEE
  IEEE COMPUTER SOC.2021: 943-946

- **Optically Induced Three-Stage Picosecond Amorphization in Low-Temperature SrTiO3.** *The journal of physical chemistry letters*
  Linker, T., Tiwari, S., Fukushima, S., Kalia, R. K., Krishnamoorthy, A., Nakano, A., Nomura, K. I., Shimamura, K., Shimojo, F., Vashishta, P.
  2020; 11 (22): 9605-9612

- **Material considerations for thermoelectric enhancement via modulation doping** *APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING*
  Beekman, M., Heaton, G., Linker, T. M., Johnson, D. C.
  2020; 126 (7)

- **Towards simulation of the dynamics of materials on quantum computers** *PHYSICAL REVIEW B*
  Bassman, L., Liu, K., Krishnamoorthy, A., Linker, T., Geng, Y., Shebib, D., Fukushima, S., Shimojo, F., Kalia, R. K., Nakano, A., Vashishta, P.
  2020; 101 (18)

- **Field-Induced Carrier Localization Transition in Dielectric Polymers.** *The journal of physical chemistry letters*
  Linker, T. M., Tiwari, S., Kumazoe, H., Fukushima, S., Kalia, R. K., Nakano, A., Ramprasad, R., Shimojo, F., Vashishta, P.
  2020; 11 (2): 352-358

- **Comparison of Predicted Thermoelectric Energy Conversion Efficiency by Cumulative Properties and Reduced Variables Approaches**
  Linker, T. M., Lee, G. S., Beekman, M.
  SPRINGER.2018: 3085-3090