Thomas M. Linker
Postdoctoral Researcher
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Contact Info:
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Education:
- 2014(Sep)-2018(June): B.S Physics, Cal Poly State University San Luis Obispo.
- 2018(Sep)-2023(May). PH.D Physics, University of Southern California.

Internships:
- June-August 2015 *Predictive Science Inc.,* San Diego CA
- June-August 2016 *Predictive Science Inc.,* San Diego CA

Successful Proposals/ Fellowships :
- DOE SCGSR 2021-2022 Doctoral Fellowship
- 2021 Cycle B Oak Ridge National Lab SNS Beam Time Proposal
- 2022 Cycle B Oak Ridge National Lab SNS Beam Time Proposal

Research Experience:

Multi Scale Machine Learning Molecular Dynamics for Large Spatiotemporal Simulations :

I have developed a multi-scale machine learning based molecular dynamics framework capable of preforming billion atom simulations with quantum mechanically accurate description of ground and excited state dynamics for studying large scale light, electrical and mechanical induced phase of materials. [1-5,10].

I developed a port of existing machine learning molecular dynamics training framework I have used at USC from Fortran to pytorch for use of the pytorch c++ API for production simulations of billion-trillion atom molecular dynamic simulations on the next generation Aurora Exa-Flop Supercomputer at Argonne National Lab as part of an Aurora Early Science Project. (https://github.com/tlinker123/torch-rx)

Nonadiabatic Quantum Dynamics for Excited States :

I have performed massively parallel non-adiabatic quantum dynamics simulations to investigate excited state dynamics of light induced topological phase transitions[3], photo-amorphization[12] and mitigating hot carrier driven dielectric breakdown in organic polymers[7,15].

Quantum Computing :

I have contributed to software development for simulation of quantum many body dynamical systems on noisy intermediate scale quantum computers and used this software to perform simulations of quantum dynamical systems on IBM and Riggeti Quantum computers [8,9,13]

Experimental Work and Collaborations :

I have worked with experimental collaborators at SLAC national lab to understand femtosecond extreme ultraviolet (XUV) transient absorption spectroscopy [11]. I have also worked with collaborators from University of Connecticut to understand how to use nano-coats to enhance the electric breakdown strength of dielectric polymers[7,15,17].

I won a DOE SCGSR fellowship as well as beam time proposal to perform neutron scattering experiments at Oak Ridge National Lab(ORNL) in conjunction with machine learning based molecular dynamics simulations to understand dynamics of quantum liquids. At ORNL I performed inelastic-neutron scattering(INS) experiments on solid and liquid ammonia and am currently writing a joint computational-experimental paper on the vibrational dynamics of ammonia based of this fellowship and beam-time experience [18]. Based off the results we submitted a proposal to study ammonia water dynamics with INS which was accepted and I completed the experiment in February 2023.

Publications:

1. **T. Linker**, K. Nomura, S., R. K. Kalia, A. Krishnamoorthy, A. Nakano, K. Shimamura, F. Shimojo, and P. Vashishta. *Nano Lett* 23, 16, 7456–7462 (2023).
2. H. Ibayashi, T. M. Razakh, L. Yang, **T. Linker**, M. Olguin, S. Hattori, Y. Luo, R. K. Kalia, A. Nakano, K. Nomura, P. Vashishta. ISC High Performance, LNCS 13948, 223-239 (2023)
3. **T. Linker**, K. Nomura, A. Aditya, S. Fukshima, R. K. Kalia, A. Krishnamoorthy, A. Nakano, P. Rajak, K. Shimmura, F. Shimojo, and P. Vashishta. *Science Advances* 8, eabk2625: 1-7 (2022)
4. **T. Linker**, K. Nomura, S. Fukushima, R. K. Kalia, A. Krishnamoorthy, A. Nakano, K. Shimamura, F. Shimojo, and P. Vashishta. *Journal of Physical Chemistry Letters* 13, 11335-11345 (2022)
5. **T. Linker**, S. Fukshima, R. K. Kalia, A. Krishnamoorthy, A. Nakano, K. Nomura, K. Shimamura, F. Shimojo, and P. Vashishta
   Frontiers in Nanotechnology **4**, 884149: 1-7 (2022)
6. J. Niman, B.S.Kamerin, T. H. Villers, **T.M. Linker**, A. Nakano, V. Kresin. *Phys. Chem. Chem. Phys*., 2022,24, 10378-10383
7. **T. Linker**, Y. Wang, A. Mishra, D. Kamal, Y. Cao, R. K. Kalia, A. Nakano, R. Ramprasad, F. Shimojo, G. Sotzing, and P. Vashishta
   ACS Applied Materials Interfaces 13, 60393-60400 (2021)

8. C. Powers, L. Bassman, **T. M. Linker**, K. Nomura, S. Gulania, R. K. Kalia, A. Nakano, and P. Vashishta
   SoftwareX 14, 100696: 1-6 (2021)
9. L. Bassman, S. Gulania, C. Powers, R. Li, **T. Linker**, K. Liu, T. K. S. Kumar, R. K. Kalia, A. Nakano, and P. Vashishta
   Quantum Science and Technology 6, 014007: 1-12 (2021)
10. P. Rajak, A. Aditya, S. Fukshima , R. K. Kalia , **T. Linker**, K. Liu, Y. Lou, A. Nakano, K. Nomura, K. Shimmura, F. Shimojo, and P. Vashishta . *2021 IEEE International Parallel and Distributed Processing Symposium Workshops* (IPDPSW), 2021, pp. 943-946, doi: 10.1109/IPDPSW52791.2021.00145.
11. R. Attar, H.-T. Chang, A. Britz, X. Zhang, M.-F. Lin, A. Krishnamoorthy, **T. Linker**, D. Fritz, D. M. Neumark, R. K. Kalia, A. Nakano, P. Ajayan, P. Vashishta, U. Bergmann, and S. R. Leone
    ACS Nano 14, 15829-15840 (2020)
12. **T. Linker**, S. Tiwari, S. Fukushima, R. K. Kalia, A. Krishnamoorthy, A. Nakano, K. Nomura, K. Shimamura, F. Shimojo, and P. Vashishta
    Journal of Physical Chemistry Letters 11, 9605-9612 (2020)
13. L. Bassman, K. Liu, A. Krishnamoorthy, **T. Linker**, Y. Geng, D. Shebib, S. Fukushima, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta
    Physical Review B 101, 184305: 1-6 (2020)
14. M. Beekman , G. Heaton, **T.M Linker** , D.C Johnson . *Applied Physics* A. 2020 Jul;126(7):1-8.
15. **T. M. Linker**, S. C. Tiwari, H. Kumazoe, S. Fukushima, R. K. Kalia, A. Nakano, R. Ramprasad, F. Shimojo, and P. Vashishta
    Journal of Physical Chemistry Letters 11, 352-358 (2020)
16. **T.M. Linker** , G.S. Lee, and M. Beekman . *Journal of Elec Materials* (2018) 47: 3085.

Publications under Review or In Preparation

17. Wang, **Linker *et al***. *Ultrahigh energy density in high-temperature polymer dielectric reinforced by bilayered nanocoating*. Under review.
18. ***Linker et al.*** *Neutron Scattering, Nuclear Quantum Effects, and Neural Networks: The Delicate Case of the Ammonia Vibrational Spectrum.* Under Review *Nature Communications.*

Oral Presentations:

1. T. Linker *et al.* ***Invited.*** Multi-Scale Neural Network Quantum Molecular Dynamics for Next Generation Energy Applications. Spetses Joint USA-European Confrence on "Extreme Scale Simulations, Machine Learning, and Neutron & X-ray Scattering for Quantum Materials" July 2023.
2. T. Linker *et al.* Multi-Scale Neural Network Molecular Dynamics Simulations for Polar Topology Control in Next Generation Ferroelectric Materials. March APS 2023.
3. T.Linker *et al. Optical Manipulation of Ferroelectric Topologies with Excited State Neural Network Quantum Molecular Dynamics.* Conference on Computational Physics 2022. Online.

4. T.Linker *et al. Multi-Scale Neural Network Quantum Molecular Dynamics Simulations for Polar Topology Control in Next Generation Ferroelectric Materials.* Materials Research Society Spring Meeting 2022 Honolulu.
5. T.Linker et al. *Mechanical Control of Ferroelectric Topologies with Hybrid Neural Network Quantum Molecular Dynamics Molecular Mechanics Simulations*. American Physical Society Conference March Meeting 2022 Chicago
6. P.Rajak, T.Linker*, et al. *Ex-NNQMD: Extreme-Scale Neural Network Quantum Molecular Dynamics.* Scalable Deep Learning over Parallel And Distributed Infrastructures 2021 Online.
7. T.Linker *et al. Finite Electron Temperature Density Functional Theory and Neural Network Molecular Dynamics study of Sub Pico-Second Optical Control of Ferroelectric Domains in $PbTiO_3$ based Nanostructures.* American Physical Society Conference March Meeting Online 2021
8. T.M Linker *et al. Non-Adiabatic Quantum Molecular Dynamics Investigation of Hot Carrier Dynamics in Dielectric Polymers under High Electric Fields.* March 2020 American Physical Society Conference Make up Meeting University of Southern California.
9. T.M Linker and M. Beekman. *Method of Four Coefficients in the Presence of Multiple Carrier Scattering Mechanisms*. March 2018 American Physical Society Conference: Thermoelectrics Focus Section. Los Angeles, CA.

* Not First Author But Presenter.

Poster Presentations:

1. Linker, T. M, Lee ,G. S, and Beekman, M. Comparing modeling approaches for estimation of thermoelectric power generation efficiency. May 2017 Cal Poly College of Science and Mathematics Research Symposium. San Luis Obispo, CA

2. Linker, T. M, Lee G. S, and Beekman, M. Cumulative Properties vs. Reduced Variables Modeling Approaches for Estimation of Thermoelectric Power Generation Efficiency. July 2017 International Conference of Thermoelectrics. Pasadena, CA.

3. Linker, T. M. and Beekman, M. Extracting Relaxation Time Scattering Parameters from Electrical Transport Data. October 2017 Frost Summer Research Symposium. San Luis Obispo, CA