Employment

Lecturer in Digital Chemistry
Lecturer
Chemistry
University of York
Heslington, York
1 Apr 2025 → present

Visiting Professor
Institute for Materials Science, TU Darmstadt
Darmstadt, Germany
1 Oct 2024 → 31 Mar 2025

Postdoc
Aalto University
Espoo, Finland
16 Sept 2022 → 30 Sept 2024

Postdoc
Ecole polytechnique fédérale de Lausanne (EPFL)
Switzerland
1 Oct 2018 → 15 Sept 2022

Qualifications

PhD, Designing a machine learning potential for molecular simulation of liquid alkanes, Department of Engineering, University of Cambridge
1 Oct 2015 → 30 Sept 2018
Award Date: 18 May 2019

Masters, Locality of forces in molecular systems, Cavendish Laboratory, University of Cambridge
1 Oct 2014 → 30 Sept 2015
Award Date: 24 Oct 2015

BSc, Stochastic simulation of genetic regulatory networks with delays
1 Sept 2010 → 31 May 2014
Award Date: 17 May 2014

Research outputs

Thermodynamics and dielectric response of $BaTiO_3$ by data-driven modeling
Gigli, L., Veit, M., Kotiuga, M., Pizzi, G., Marzari, N. & Ceriotti, M., 29 Sept 2022, In: npj Computational Materials. 8, 1, 17 p., 209.

Roadmap on Machine learning in electronic structure
Kulik, H. J., Hammerschmidt, T., Schmidt, J., Botti, S., Marques, M. A. L., Boley, M., Scheffler, M., Todorović, M., Rinke, P., Oses, C., Smolyanyuk, A., Curtarolo, S., Tkatchenko, A., Bartók, A. P., Manzhos, S., Ihara, M., Carrington, T., Behler, J., Isayev, O. & Veit, M. & 27 others, Grisafi, A., Nigam, J., Ceriotti, M., Schütt, K. T., Westermayr, J., Gastegger, M., Maurer, R. J., Kalita, B., Burke, K., Nagai, R., Akashi, R., Sugino, O., Hermann, J., Noé, F., Pilati, S., Draxl, C., Kuban, M., Rigamonti, S., Scheidgen, M., Esters, M., Hicks, D., Toher, C., Balachandran, P. V., Tamblyn, I., Whitelam, S., Bellinger, C. & Ghiringhelli, L. M., 19 Aug 2022, In: Electronic Structure. 4, 2, 61 p., 023004.

Efficient implementation of atom-density representations
Musil, F., Veit, M., Goscinski, A., Fraux, G., Willatt, M. J., Stricker, M., Junge, T. & Ceriotti, M., 16 Mar 2021, In: Journal of Chemical Physics. 154, 11, 17 p., 1141091.

Predicting molecular dipole moments by combining atomic partial charges and atomic dipoles
Veit, M., Wilkins, D. M., Yang, Y., Distasio, R. A. & Ceriotti, M., 9 Jul 2020, In: Journal of Chemical Physics. 153, 2, 14 p., 024113.

Multi-scale electrolyte transport simulations for lithium ion batteries
Hanke, F., Modrow, N., Akkermans, R. L. C., Korotkin, I., Mocanu, F. C., Neufeld, V. A. & Veit, M., 22 Nov 2019, In: Journal of the Electrochemical Society. 167, 1, 4 p., 013522.

Equation of State of Fluid Methane from First Principles with Machine Learning Potentials
Veit, M., Jain, S. K., Bonakala, S., Rudra, I., Hohl, D. & Csányi, G., 9 Apr 2019, In: Journal of chemical theory and computation. 15, 4, p. 2574-2586 13 p.

Datasets

Models and source data for MuML dipole fitting
Veit, M. (Creator), Wilkins, D. M. (Creator), Yang, Y. (Creator), DiStasio Jr, R. A. (Creator) & Ceriotti, M. (Creator), Zenodo, 11 May 2020
DOI: 10.5281/zenodo.3820297, https://zenodo.org/record/3820297

Quantum mechanical dipole moments in the QM7b, 21k molecules of QM9, and MuML showcase datasets
Veit, M. (Creator), Wilkins, D. M. (Creator), Yang, Y. (Creator), DiStasio Jr, R. A. (Creator) & Ceriotti, M. (Creator), Materials Cloud, 10 Jun 2020
DOI: 10.24435/materialscloud:2k-3h, https://archive.materialscloud.org/record/2020.56

Thermodynamics and dielectric response of $BaTiO_3$ by data-driven modeling
Gigli, L. (Creator), Veit, M. (Creator), Kotiuga, M. (Creator), Pizzi, G. (Creator), Marzari, N. (Creator) & Ceriotti, M. (Creator), Materials Cloud, 29 Jun 2022
DOI: 10.24435/materialscloud:9g-k6, https://archive.materialscloud.org/record/2022.88