Poster Titles and Numbers

1	**Bridging the Gap: Integrating Machine Learning with Quantum Mechanical Calculations for Enhanced Molecular Electrostatics Modelling** *Charlie Adams, Josh Horton, David Wright, Daniel Cole*
2	**Protein dynamics and the temperature adaptation of enzyme catalysis: simulations of wild type and mutants MalL** *Marvellous Arabambi , Carlin J Hamill, Vickery L Arcus, Marc van der Kamp, Frank Vollmer and Adrian J Mulholland*
3	**Multi-Scale Theoretical Investigation of the Linear and Nonlinear Optical Responses of Di-8-ANEPPS Embedded in Complex Environments: on the Way to Explore the Complexity of Cell Membranes** *Charlotte Bouquiaux, Tarcius N. Ramos, Pierre Beaujean, Frederic Castet, Benoit Champagne*
4	**Time-dependent study of light-induced hapticity changes in a ruthenium sandwich complex** *Vera Brieskorn, Basile Curchod*
5	**Direct dynamics simulation of prospective PFAS molecules dissociation after electron impact of PPVE and C4H3F7O isomers.** *Ryan Brook, Dmitry Makhov, Dmitry Shalashillin*
6	**Shapespyer: a Python driven toolchain for soft matter simulations** *Andrey Brukhno, Michael Seaton, John Purton, Tim Snow and James Doutch*
7	**Exploring Cluster Surface Adsorption: A Proof-of-Concept Investigation of Phase Space Volume Using Nested Sampling** *Thanawitch Chatbipho, Mingrui Yang, Robert B. Wexler, Livia B. Partay*
8	**Simulating Nonadiabatic Dynamics Using the Meyer-Miller-Stock-Thoss Hamiltonian: A Comparison of Algorithms** *Lauren E. Cook, Johan E. Runeson , Jeremy O. Richardson , and Timothy J. H. Hele*
9	**Isolated cyanovinyl anion as a potential stable synthon** *Adrianna Cyraniak, Iwona Anusiewicz, Sylwia Freza, Piotr Skurski*
10	**Exploring Intermolecular Induction through Non-Orthogonal Pauli-Blockade Framework** *Humahuti Dihingia, Bartosz Tyrcha, Piotr S. Zuchowski, Alston J. Misquitta*
11	**Improving Gaussian Basis Sets for Molecules with Machine Learning** *Shaun T. E. Donnelly, J. Grant Hill*
12	**mol-CSPy: An open-source crystal structure prediction code** *G. M. Day, J. Bramley, P. W. V. Butler, P. J. Bygrave, D. H. Case, C. Y. Cheng, R. Cuadrado, J. Dickman, J. Dorrell, J. Glover, R. Hafizi, J. Johal, D. P. McMahon, J. Nyman, P. R. Spackman, C. R. Taylor, J. Yang, and S. Yang*

13	**Predicting Absorption and Emission Spectra of Solvated Nile Red with ESTEEM** *Nicholas Hine, Jacob Eller, Panos Kourtis, Carlo Maino*
14	**Spin-Dependent Nonorthogonal Generalised Wannier Functions for Linear-Scaling Density Functional Theory** *Miguel Escobar-Azor, Ali Safavi , David O'Regan , Nicholas D. M. Hine*
15	**Contact Map Path Sampling for Protein Folding** Ziad Fakhoury, Gabriele Sosso, Scott Habershon
16	**Understanding Conformational Free Energy Surfaces through Enhanced Sampling Molecular Dynamics and Unsupervised Clustering Methods** *Alexandre Ferreira, Matteo Salvalaglio, Ivan Marziano, Rui Guo*
17	**Catalytic Partial Oxidation of Methane using an Yttria-Stabilized Zirconia** *Erze Gao, Alexey Sokol, Richard Catlow*
18	**Fast, accurate and spin-pure calculation of the electronically excited states of radicals** *James D. Green, Jingkun Shen, Keith T. Butler, Timothy J. H. Hele*
19	**Electron tunnelling and vibrational relaxation rates for chemisorbed hydrogen on metals from Projector Operator Diabatisation** *Nils Hertl, Zuszsanna Konczor-Benda , Reinhard J. Maurer*
20	**Insight into the Correlated Disorder of Fumarate-Based MIL-53 Frameworks: A Computational Study of Free-Energy Landscapes** *Chi Cheng Hong, Ross S. Forgan, Antonia. S. J. S. Mey, Claire L. Hobday*
21	**Point charge embedding approaches for simulating excited states in MOFs** *Michael Ingham, Amir Sidat , Alex Aziz, Devis Di Tommaso, Rachel Crespo-Otero*
22	**Nanoscale Non-adiabatic Dynamics Simulation of Charge Generation in Organic Solar Cells** *Filip Ivanovic, Samuele Giannini, Jochen Blumberger*
23	**Electronic structure of the InAs-Al interface via DFT: using ZnTe and CdSe barriers for topological devices** *Malcolm J.A. Jardine, Derek Dardzinski, Chris J. Palmstrom, Moira Hocevar, Vladimir N. Strocov, Sergey M. Frolov, Noa Marom*
24	**L1 Metallo-$\hat{1}^2$ -Lactamase Antimicrobial Resistance Enzyme: A Computational Reaction Mechanism Study** *Papu Kalita, Philip Hinchliffe, James Spencer, Adrian J. Mulholland*
25	**Modelling Excited State Dynamics of Organic Materials in the Condensed Phase** Karolina Kapusta, Rachel Crespo-Otero

Poster Titles and Numbers

26	**Covalent Organic Frameworks for Drug Delivery** *Gregor J. Lauter, Alessandro Calzolari, Ganna Gryn'ova*
27	**Copper Nanowires for Electrochemical CO2 Reduction Reaction** *Wuyang Lin, Azeem Ghulam Nabi, Matteo Palma, and Devis Di Tommaso*
28	**Nonadiabatic Energy Loss During Hydrogen Scattering on Semiconductors** *Xuexun Lu, Sara Oregioni, Nils Hertl, Reinhard J. Maurer*
29	**Automating transition state search in metal catalysed reactions** *Shoubhik R. Maiti, Fernanda Duarte, David Buttar*
30	**Machine Learning-Driven Virtual Screening for Antibacterial Design Targeting Enoyl-ACP Reductase (FabI)** *Veríssimo, G.C. ; Kronenberger, T.; Costa, D.M.A.; Maltarollo, V.G.*
31	**ichor: A Python library for computational chemistry data management and machine learning force field development** *Yulian T. Manchev, Matthew J. Burn, and Paul L. A. Popelier*
32	**Alchemical free energy calculations using machine learned forcefields** *J. Harry Moore, Gabor Csanyi*
33	**Electrolyte dynamics with potential-induced charges on electrodes: Implementation and usage as a starting point for DFT calculations.** *Sara Navarro, Federico N. Pedron, Pablo Ordejón*
34	**Unravelling nucleation in Ferritin nanocages from atomistic molecular dynamics simulations** *Matteo Paloni, Johanna Galloway, Aaron R. Finney, Fiona Meldrum, Matteo Salvalaglio*
35	**Investigating conductive properties of a single-heme cytochrome** *András Pethő, Jochen Blumberger*
36	**In search of enzyme activation: A steered molecular dynamics/Markov state model workflow for evaluating allosteric drug candidates** *Frederick Powell, Adele Hardie, Dr Graeme Barker, Julien Michel*
37	**The comparative assessment of linear and nonlinear Hamiltonian models** *Chen Qian, Reinhard Maurer*
38	**Investigating allosteric inhibitory mechanisms of the soluble epoxide hydrolase** *Qiongju Qiu, Franca Fraternali and Maria R. Conte*

39	**Tuning Zeolite Catalysts using Organic Additives** *Matt Robinson, Andrew Logsdail*
40	**Understanding Organic Cocrystals for Room Temperature Phosphorescence** *Kanyarat. Rueangboon, Maria Eugenia. Sandoval-Salinas, Rachel. Crespo-Otero*
41	**Theoretical Electronic Structure of Iron(III)-Oxo Clusters** *Ali Safavi, Nicholas Hine*
42	**The role of structural isomers in the photophysics of organic crystals** *Maria Eugenia Sandoval-Salinas, Federico J. Hernandez, Rachel Crespo-Otero*
43	**Exploration of Defect Superstructures in Graphene** *Benedict Saunders, Lukas Hörmann, Reinhard J. Maurer*
44	**Non-equilibrium electrons generated from the extended two-temperature model to drive chemical dynamics at surfaces** *Henry T. Snowden, Reinhard J. Maurer*
45	**Molecular dynamics investigation of the role of lattice heating in laser-driven hydrogen evolution at copper surfaces** *Alexander Spears, Wojciech G. Stark, Reinhard J. Maurer*
46	**Nonadiabatic effects in reactive hydrogen dynamics at Cu surfaces** *Wojciech G. Stark, Connor L. Box, Reinhard J. Maurer*
47	**Effective Harmonic Potential Study of Mg Interstitials Using Neural Network** *Zhuoyang Ti, Georg K. H. Madsen*
48	**Developing Standardised Modelling Workflows for QM/MM Studies of Metal Oxides** *O. van Vuren, G. A. Bramley, A. J. Logsdail*
49	**Computational Approach for Targeting Serine Protease Inhibitors in Oral Cancer: Insights into Serpin Expression Dynamics and Drug Design** *Soujanya Jagadish Vastrad, Saraswathy Ganesan Rajalekshmi, Ashok Madarkhandi*
50	**Modelling the Dermal Absorption of Agrochemicals** *Callum Ward, Conor Whitehouse, Jennifer Webb and Rebecca Notman*
51	**Elucidating the role of potassium in methane steam reforming using first-principles-based kinetic Monte Carlo simulations** *Sai Sharath Yadavalli, Carlo Fonte, Glenn Jones and Michail Stamatakis*