RESEARCH CONFERENCES

ESF-LFUI Conference
Energy Landscapes
Obergurgl Austria

# LIST OF ACCEPTED POSTERS

| Poster Number | Surname | Firstname | Poster Title |
|---|---|---|---|
| 1 | Antlanger | Moritz | Ordered structures in dipolar, layered systems |
| 2 | Bakaeva | Zulfiya | Critical behavior of nanoparticle-containing binary liquid mixtures |
| 3 | Baldock | Robert John Nicholas | Nested Sampling - an efficient, unbiased method for finding the partition function of a system as an explicit function of temperature. |
| 4 | Deckman | Jason | Quantum Induced Structural Transformations in Lennard-Jones Clusters. |
| 5 | Dieterich | Johannes | Explorations of accurate and not-so-accurate energy landscapes |
| 6 | Do | Hainam | A DFT Basin Hopping Study of Small Water, Methanol and Water Plus Methanol Clusters |
| 7 | Doppelbauer | Günther | Ordered equilibrium structures formed by patchy particle systems. |
| 8 | Farrell | James Daniel | Benchmarking global minimisation algorithms |
| 9 | Fiser | Béla | Glutahione as an Ancient Prebiotic Peptide |
| 10 | Flikkema | Edwin | Global optimization studies of silica clusters and hydroxylated silica clusters. |
| 11 | Forman | Chris | Design principles for helical bilayered fibres |
| 12 | Grebner | Christoph | Tabu Search Based Global Optimization Algorithms for Problems in Computational Chemistry |
| 13 | Heard | Christopher | Empirical and DFT energy landscapes of bimetallic coinage metals |
| 14 | Hédin | Florent Henri René | Sampling Rare Events with Spatial Averaging: Implementation and Application to Rare Gas Clusters and Biomolecules |
| 15 | Hoffmann | Falk | Protein structure prediction using basin-hopping with NMR chemical shift restraints |
| 16 | Joly | Jean-Francois | The stability of vacancy-like defects in amorphous silicon, a kinetic ART study |
| 17 | Kaneko | Toshihiro | Size-Dependent Phase Transitions in TIP4P Water Clusters Investigated by Multicanonical-Ensemble Molecular Dynamics Simulations |
| 18 | Kusumaatmaja | Halim | Defect Motifs on Constant Mean Curvature Surfaces |
| 19 | Moebius | Arnulf | On parallelization of structure optimization via local heat pulse - quench cycles employing the GULP code |

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| Poster Number | Surname | Firstname | Poster Title |
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| 20 | Nagai | Tetsuro | Application of Simulated Tempering and Magnetizing (STM) to the Ising Model |
| 21 | Neelamraju | Sridhar | Ab initio and empirical energy landscapes of (MgF2)n clusters (n = 3, 4). |
| 22 | Nerukh | Dmitry | Combined peptide-water energy landscape: the dynamics of rare conformational transitions |
| 23 | Nicolaï | Adrien | Deciphering the conformational changes induced by ATP binding in a HSP70 molecular chaperone from an analysis of its free-energy landscape in different nucleotide states. |
| 24 | Oakley | Mark | Energy Landscapes of Cyclic Peptides |
| 25 | Olesen | Scott W. | A novel design principle for chiral structures |
| 26 | Owen | Michael | Free radical-initiated unfolding of peptides using energy landscape methods. |
| 27 | Radu | Liliana | Fluorescence resonance energy transfer, time resolved spectroscopy and precision calorimetry as additional methods to energy landscapes for chromatin dynamic structure determination |
| 28 | Ruehle | Victor | Exploring crystal energy landscapes |
| 29 | Ruzicka | Stepan | Virtual Move Monte Carlo: Full Symmetrization; Folding kinetics of a flexible homopolymer chain |
| 30 | Sevink | Geert Jan Agur | Efficient multi-scale simulation with the Stochastic Quasi-Newton method |
| 31 | Shalashilin | Dmitry | Describing short and long time dynamics of peptides with Boxed Classical Dynamics |
| 32 | Singh | Priya | Performance of Wang-Landau algorithm and accurate calculation of density of states near ground state for bio molecules |
| 33 | Smeeton | Lewis Conrad | Visualisation of Energy Landscapes |
| 34 | Somani | Sandeep | Comparison of equilibrium sampling and energy landscape based methods of computing thermodynamic quantities of biomolecules |
| 35 | Sopu | Daniel | Nanoglasses: an approach to improve the plastic behavior of metallic glasses |

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| Poster Number | Surname | Firstname | Poster Title |
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| 36 | Uhrin | Martin | Why are particular crystal structures stable over others? Insights from the binary Lennard-Jones system |
| 37 | Várnai | Csilla | Exploring the energy landscapes of protein folding simulations with Bayesian computation |
| 38 | Yurtsever | Ersin | Structures, Dynamics and thermodynamics of trapped ionic clusters |
| 39 | Zeravcic | Zorana | You can always get what you want |