Journal of Innovative Materials in Extreme Conditions
2020
Volume 1
Issue 1

ENERGY LANDSCAPES 2019

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Abstract: *This article summarizes the presentations delivered at the Energy Landscapes Conference held in Belgrade, Serbia, from 26 to 30 August 2019. The focus of the conference was on the present state of the art in theoretical energy landscape approaches, and their applications in the fields of chemistry, physics, biology, and materials science in general. The presentations were organized around some of the hot topics, such as applications from spectroscopy to the solid-state, folding and misfolding of proteins, DNA and RNA, multiscale modeling, materials under extreme pressure/temperature conditions, designing landscapes for self-assembly and multifunctional systems, landscapes for machine learning, atomic, molecular, colloidal and nanoalloy clusters.*

Keywords**:** *energy landscapes, multiscale modeling, extreme pressures, high temperature, structure prediction, biomolecules, nanostructures, proteins, theoretical methods*

1. Introduction

The energy landscape workshops originated in Telluride (USA), where since the mid-1980's specialized workshops about e.g. structures and dynamics of clusters, global optimization methods, modern thermodynamics, and dynamics of proteins, have taken place. During these workshops, short presentations followed by long in-depth discussions (typical ratio: 1:3) allowed researchers from different sub-fields to closely interact and form new alliances; frequently new collaborations were born or papers were conceived and partly written as an outcome of these discussions.

In the mid-nineties, it became clear that all these topics were intimately connected with complex energy landscapes but that different research communities were often unaware of the progress in other groups, regarding the underlying energy landscape concepts. Thus, it was decided to start a dedicated workshop series on energy landscapes every one or two years, with the first one taking place in 1997, which were aimed at researchers from a wide variety of fields, ranging from computer science over physics and chemistry to biology and beyond. Originally all meetings took place at the Telluride Science Research Center (TSRC) in Telluride, U.S.A. [1], but in 2000, an energy landscape workshop took place in Europe (Chemnitz, Germany), and since 2007 (Petritoli, Italy) [2-7], workshops have more or less alternated between Telluride and Europe, with one workshop taking place in India (Goa, 2017) as well [8].

2. Conference Summary

This Energy Landscapes Conference was held in Belgrade, Serbia, from 26 to 30 August 2019. The focus of the meeting was on the present state of the art in theoretical energy landscape approaches and their applications in the fields of chemistry, physics, biology, and material science in general. The conference was organized around the morning and afternoon sessions, with afternoon breaks for a guided walking tour and a visit to the Tesla museum. The presentations were organized around some of the hot topics, such as applications from spectroscopy to the solid state, folding and misfolding of proteins, DNA and RNA, multiscale modeling, designing landscapes for self-assembly and multifunctional systems, landscapes for machine learning, atomic, molecular, colloidal and

nanoalloy clusters, and molecules on surfaces. Presentations were all contributed talks of 25 minutes with 10 minutes discussion, and posters [9,10].

Figure 1. A group photo of the participants of the Energy Landscape 2019 in the conference hall.

The Energy Landscapes 2019 meeting consisted of twenty-five oral presentations and eight poster presentations. A group photo of the participants is shown in Figure 1. The scientific sessions were followed by guided city walking tours and a visit to the Nikola Tesla science museum (Figure 2). We would like to note the gender balance of the conference since 30% of all presentations were contributions from female participants, which we aim to increase in the future [11]. We would also like to point to the great variety of participating countries, ranging from the U.S.A. to New Zealand, including Germany, India, China, Israel, Luxemburg, France, Romania, the United Kingdom, and Serbia. Furthermore, participants included representatives from top-ranked institutions and universities of the participating countries. A sizable fraction of the participants came from the University of Cambridge (United Kingdom) and the Institute of Nuclear Sciences "Vinča" (Serbia), which was expected, since the conference was organized by **David J. Wales** and **Dejan B. Zagorac** from these institutions.

After arrival and official welcome reception on Monday, the oral presentations started on Tuesday with opening remarks *Welcome to Energy Landscapes 2019*, given by one of the organizers, **David J. Wales**, from the University of Cambridge (UK). This introduction was followed by an oral presentation by **Biman Bagchi**, from the Indian Institute of Science, Bangalore, India, talking about the *free energy landscape of insulin dimer dissociation*. The next talk was given by **Vladimir Mandelshtam**, the University of California, Irvine, USA, presenting *quantum-induced disordering in anionic hydrogen and deuterium clusters*, followed by a talk from **Atreyee Banerjee**, University of Cambridge, UK, presenting *Crystal Structure Prediction for Benzene Using Basin-Hopping*. After a coffee break, **Karl Heinz Hoffmann**, from the Technical University Chemnitz, Germany, presented *Preferential Trapping and Controlled Dynamics on Energy Landscapes*.

The morning session finished with the talk: *Finding low-lying minima structures of Au and Pt nanoclusters*; given by **Anna Garden** from the University of Otago, Dunedin, New Zealand. The afternoon session consisted of the oral presentations given by **Maria Čebela**, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, on *Bismuth ferrite (BiFeO3): A multidisciplinary approach to multiferroics*, and **Snežana Zarić**, from the Faculty of Chemistry, University of Belgrade, Serbia, presenting *Energy landscapes of aromatic/aromatic interactions*.

Wednesday (28th of August) started with the talk: *Algorithms which aim at fast bracketing interval reduction for the solution of nonlinear equations and one-dimensional minimization: how answering a simple question leads to simultaneously highly efficient and very robust procedures*, given by **Arnulf Moebius**, IFW- Leibniz Institute for Solid State and Materials Research Dresden, and TU Chemnitz, Germany. It was followed by a lecture *Exploring energy landscapes of reactive condensed-phase systems*, given by **David Furman**, from the University of Cambridge, UK. The next talk was given by **Vladimir Damljanović**, Institute of Physics, Belgrade, Serbia, with the title: *The connection between electronic dispersions and symmetries of two- and three-dimensional single*

crystals. After the coffee break, **Igor Pašti**, from the Faculty of Physical Chemistry, University of Belgrade, Serbia, gave a talk on *reactivity of graphene basal plane around point defects and surface functional groups.* The last talk of the morning session was given by **Christian Schön**, Max Planck Institute for Solid State Research, Stuttgart, Germany, with the title: *Energy landscape explorations of molecules in vacuum and on surfaces*.

Figure 2. The conference logo, participants of Energy Landscapes 2019 visiting the Tesla Museum, and the conference dinner (read from the anti-clockwise).

Wednesday afternoon was a poster session, consisting of posters by **Jelena Luković**, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, with the title: *Synthesis, Characterization, and Prediction of New Crystal Structures of WSi_2 using ab initio data mining approach*; **Manuel Perez Jigato**, Luxembourg Institute of Science and Technology, Luxembourg, with the title: *The $CuBO_2$ conundrum: neither delafossite nor monoclinic;* two posters by **Tamara Škundrić**, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, with the titles: *Structure prediction and energy landscapes of the novel CrSiN system;* and *Energy landscapes of ZnO on atomic scale;* **Maria Čebela**, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, with the title: *Structural and magnetic properties of holmium doped $BiFeO_3$*; **Geoffrey Weal**, University of Otago, Dunedin, New Zealand, with the title: *Using a CNA-based structural comparison method to improve the efficiency of the genetic algorithm*; **Qiang Zhu,** Nanjing University, Jiangsu, China, with the title: *A Data-Driven Accelerated Sampling Method for Searching Functional States of Proteins*; and **Dušica Jovanović**, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, with the title: *Theoretical investigations of pristine and doped TiO_2 using DFT.*

The morning session on Thursday 29th started with the oral presentation *A minimalistic model for nanoscale closed-shell structures based on ionic interactions: Goldberg shells and beyond* given by **Szilard Fejer**, from the Promedical Center, Cluj-Napoca, Romania. It was followed by the talk *Autonomous exploration of defective crystal energy landscapes using kinetic uncertainty measures* given by **Tom Swinburne**, CINaM - Centre Interdisciplinaire de Nanoscience de Marseille, France, and the talk *Multifunctional nanodevice based on a TiO_2 monolayer* given by **Igor Popov**, from the Institute of Physics, Belgrade, Serbia. After the coffee break, **Ben Shires**, University of Cambridge, UK, gave an oral presentation: *Visualising energy landscapes using stochastic neighbour embedding*. The Thursday morning session concluded with *Evolutionary free energy landscape of Ag-Au compositional alloys*, given by **Dasari L. V. K. Prasad**, from the Indian Institute of Technology Kanpur, Kanpur, India. The afternoon session consisted of two lectures, the first, *Pasta, viruses and chiropoles: a novel coarse-grained chiral potential*, given by **John Morgan**, University of Cambridge, UK, and, the second, *The metal-insulator transition in disordered solids: How theoretical*

prejudices influence its characterization: A critical review of analyses of experimental data, given by **Arnulf Moebius**, from the IFW- Leibniz Institute for Solid State and Materials Research Dresden, and TU Chemnitz, Germany.

The last day of the conference (Friday 30th) started with the lecture *Energy landscapes of some knotted proteins*, given by **Sridhar Neelamraju**, University of Cambridge, UK. It was followed by **Asem Hassan**, Northeastern University, Boston, U.S.A., with the title: *Describing collective motions in a large biomolecular assembly.* The next oral presentation, *Local ab initio optimizations of globally predicted CeON compound using empirical potentials*, was given by **Jelena Zagorac**, from the Institute of Nuclear Sciences "Vinča", Belgrade, Serbia. After the coffee break, **Alasdair Keith**, University of Cambridge, UK, gave a talk: *Using the Energy Landscape to Elucidate Protein-Ligand Interactions*. The last talk and closing remarks were given by one of the organizers, **Dejan Zagorac**, Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, with the title: *Structure prediction and energy landscape investigations of* $ZnO_{1-x}S_x$ *solid solutions using threshold algorithm and PCAE method*.

3. Conference news and announcements

Our dear friend and colleague, Professor Roy Johnston, 58, has passed away after a long illness [12]. He was a Professor of Computational Chemistry at the University of Birmingham and a regular attendee of Energy Landscapes conferences. All those who have worked and interacted with him, all his friends, and colleagues, will deeply miss him.

The next Energy Landscape 2020 workshop with the title "Energy Landscapes: Structure, Dynamics and Exploration Algorithms" is planned at the Telluride Science Research Center (TSRC) for the period August 3rd - August 7th, 2020 organized by Janett Prehl, Karl Heinz Hoffmann, and Christian Schön. The workshop will be devoted to a discussion of systems with multi-minima energy landscapes, such as glasses, crystalline solids, proteins, clusters, large molecules, and combinatorial optimization problems. More information is available here [13].

We also want to point out that in the week before, a closely related workshop on "Optimization of thermodynamic systems" is organized by Karl Heinz Hoffmann and Peter Salamon (July 27th – July 31st, 2020). We would like to welcome a number of the participants of the landscapes workshop there as well (and conversely) to allow and support additional discussions and perhaps the development of research projects beyond the time available during the first week. Therefore, we recommend joining us for both weeks. More information is available here [14].

Acknowledgments

The authors would like to thank L. Masters, J. Zagorac, M. Čebela, J. Luković, T. Škundrić, D. Jovanović, and B. Matović for helping to organize the conference. The following funding is acknowledged: Ministarstvo Prosvete, Nauke i Tehnološkog Razvoja (grant No. 45012), and the Royal Society of Chemistry.

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