Seminarium NOMATEN

wtorek 09.02.2021 godz. 13:00-15.00

https://www.gotomeet.me/NCBJmeetings/nomaten-seminar

Dr Elena Akhmatskaya

(Ikerbasque Foundation Professor and a Group Leader at Basque Center for Applied Mathematics - Bilbao, Basque Country, Spain)

Dr Elena Akhmatskaya is an Ikerbasque Professor and a Group leader at the Basque Center for Applied Mathematics (Bilbao, Basque Country, Spain), as well as an Affiliate Research Professor at the Berkeley Lab (USA). She is an applied mathematician, whose scientific interests include designing numerical algorithms for quantum, atomistic, meso- and multiscale simulations, their implementation in the software and subsequent application to the frontline research in Life and Physical Sciences using High Performance Computers.

In addition to her international academic experience in the USA (Cornell University), the UK (University of Manchester, Imperial College London), Spain (BCAM) she has spent 13 years working at Fujitsu, UK as Principal Researcher. She is an author/co-author of 8 European/GB/US patents, 90+ articles (including a paper with 1400+ citations) in multi-disciplinary scientific journals, 3 commercial and 4 open source software packages, with applications in high performance computing.

Elena is a Review Editor on the Editorial Board of *Physical Chemistry and Chemical Physics* (specialty section of Frontiers in Chemistry and Frontiers in Physics).

Abstract: Mathematically Enhanced Atomistic Simulation of Advanced Energy Materials

Development of efficient strategies for the rational design of materials involved in the production and storage of renewable energy is essential for accelerating the transition to a low-carbon economy. To contribute to this goal, we propose a novel workflow for assessment and optimization of battery materials. The approach effectively combines quantum and atomistic modelling/simulations, enhanced by efficient sampling, Bayesian parameterization and experimental information. It is implemented to study prospective materials for lithium and sodium batteries.

Mathematically Enhanced Atomistic Simulation of Advanced Energy Materials: Elena Akhmatskaya[1, 2], Mauricio R. Bonilla[1], Fabian Garcia[3], Carlos Leon Chinchay[1], Javier Carrasco[4]

[1]*BCAM - Basque Center for Applied Mathematics, Alameda de Mazarredo 14, E-48009 Bilbao, Spain*

[2]*IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, E-48009 Bilbao, Spain*

[3]*Department of Chemical Engineering and Analytical Science, The University of Manchester, Manchester M13 9PL, United Kingdom*

[4]*Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Alava Technology Park, Albert Einstein 48, 01510, Vitoria-Gasteiz, Spain*