Olexandr Isayev

Assistant Professor, Chemistry at Carnegie Mellon University

Pittsburgh, PA, US

Olexandr Isayev's research focuses on solving fundamental chemical problems with machine learning, molecular modeling and quantum mechanics.

Biography

Working to connect artificial intelligence with chemical sciences, Olexandr Isayev's research focuses on solving fundamental chemical problems with machine learning, molecular modeling and quantum mechanics. his lab works at the interface of theoretical chemistry, pharmaceutical sciences and computer science, working in such areas as theoretical and computational chemistry, machine learning, cheminformatics, drug discovery, computer-aided molecular design and materials informatics.

Industry Expertise

Education/Learning, Pharmaceuticals, Chemicals

Areas of Expertise

Theoretical Chemistry, Computational Chemistry, Machine Learning, Cheminformatics, Drug Discovery, Computer-aided Molecular Design, Materials Informatics

Education

Dnepropetrovsk National University M.S. Chemistry

Jackson State University
Ph.D. Theoretical Chemistry

Accomplishments

Eshelman Institute for Innovation Award 2016

Chemical Structure Association Trust Award 2015

NVIDIA GPU Computing Award 2014

IBM-Löwdin Memorial Fellowship 2009

ACS Emerging Technology Award 2017, 2014

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