AVVISO SEMINARIO

Il giorno Venerdì 8 Marzo 2024
alle ore 11:00 nell'aula G del
dipartimento di Chimica, Biologia e Biotecnologie

Prof. Loriano Storchi

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Terrà un seminario dal titolo:

CLASSIFICATION OF BIOMOLECULAR STRUCTURES BY INVARIANT SHAPE AND DEFORMATION PARAMETERS

We will present an overview of Machine and Deep Learning techniques applied in two different scenarios. Specifically, Deep Learning approaches are able to automatically extract relevant features from the input data and capture nonlinear relationships between the input and output. We present the GRID-derived AI (GrAId) descriptors, a simple modification to GRID MIFs that facilitate their use in combination with Convolutional Neural Networks (CNNs) to build Deep Learning models in a rotationally, conformationally, and alignment-independent approach we are calling DeepGRID [1]. On the other end, we propose a combinatorial machine-learning approach to obtain physical formulas based on simple and easily accessible ingredients, such as atomic properties. The latter are used to build materials features that are finally employed, through linear regression, to predict the energetic stability of semiconducting binary compounds with respect to zinc blende and rocksalt crystal structures. The adopted models are trained using a dataset built from first-principles calculations [2].

[1] Loriano Storchi, Gabriele Cruciani, Simon Cross, "DeepGRID: Deep Learning using GRID descriptors for BBB prediction", Journal of Chemical Information and Modeling, DOI: 10.1021/acs.jcim.3c00768 (2023)
[2] Udaykumar Gajera, Loriano Storchi, Danila Amoroso, Francesco Delodovici, Silvia Picozzi "Towards machine learning for microscopic mechanisms:a formula search for crystal structure stability based on atomic properties" Journal of Applied Physics, DOI: 10.1063/5.0088177 (2022)

. Tutti gli interessati sono invitati a partecipare

Dott. Giovanni Bistoni