CeCBiD-EOSC

Nanoscience

Obiectiv: Realizarea de servicii si aplicatii informatice pentru suportul activitatii de modelare si simulare a nanostructurilor.

Activitati:

1. Instalarea pachetelelor software dedicate calculelor de tip *ab initio* **(SIESTA, ABINIT, Quantum ESPRESSO)**, dinamica moleculara **(LAMMPS)**, pachete/librarii destinate segmentului de invatare automata (machine learning - ML): **TensorFlow, Keras, PyTorch, Scikit-learn** etc si de implementare a algoritmilor evolutivi **(CALYPSO)**.

2. Calcule folosind **teoria functionalei de densitate (DFT)** pentru determinarea proprietatilor electronice (e.g. largimea benzii interzise), optice (e.g. coeficient de absorbtie), mecanice (e.g. modul de elasticitate, duritate) in materiale nanostructurate.

3. Implementarea si testarea **retelelor neurale artificiale** pentru predictia proprietatilor de material (mixturi grafena – nitrura de bor hexagonala, aliaje cu entropie ridicata / high entropy alloys).

4. Aplicarea **algoritmilor evolutivi** pentru design-ul de noi materiale (optimizarea duritatii).

5. Implementarea modelor de **dinamica moleculara**: transport de ioni, nanoindentare etc.

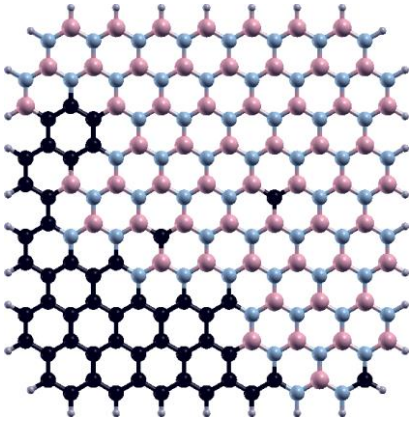
6. Studiul **dispozitivelor neurale cuantice**.

Aplicatii DFT

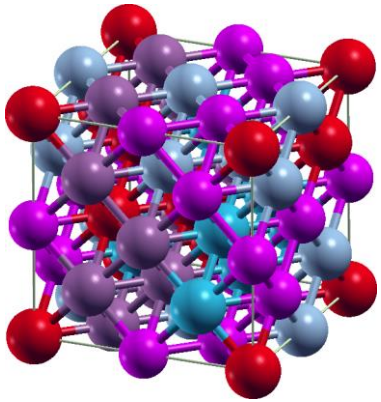
SIESTA: Spanish Initiative for Electronic Structure with Thousands Atoms

Caracteristici:
- Scalare liniara a timpul de calcul cu numarul de atomi, prin utilizarea setului de elemente de baza strict localizate (orbitali numerici atomici).
- Implementare MPI: F. Corsetti, *Performance Analysis of Electronic Structure Codes on HPC Systems: A Case Study of SIESTA*, PLOS ONE 9, e95390 (2014).

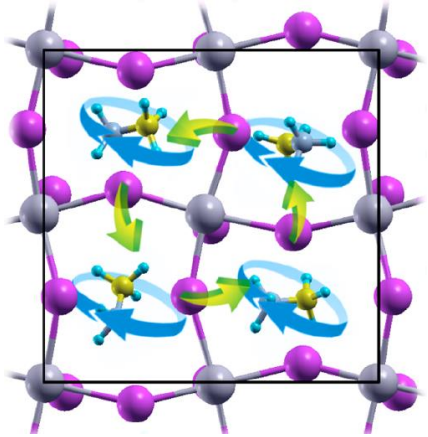
Sisteme investigate:



Sisteme hibride grafena – nitrura de bor hexagonala



Aliaje cu entropie ridicata (HEA)
E.g. CoCrFeNiAl



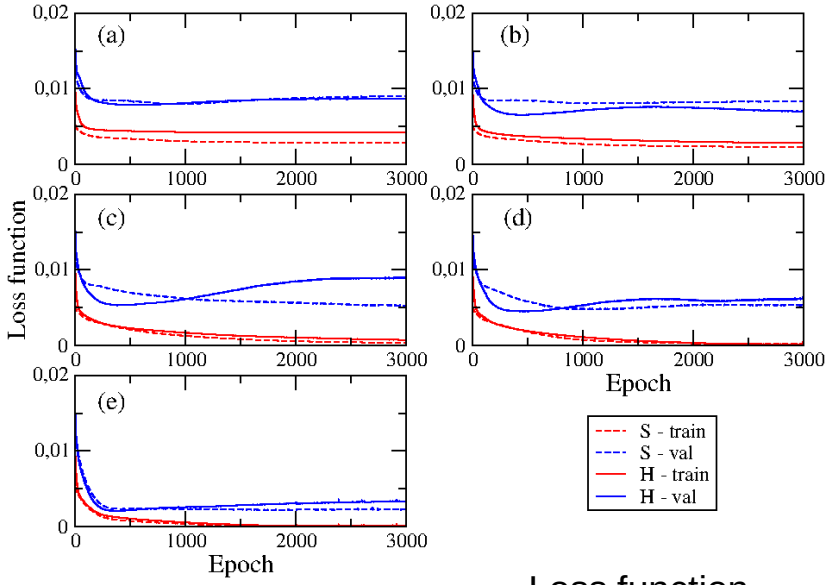
Perovskiti hibrizi
(organic-anorganic)

Retele neurale artificiale

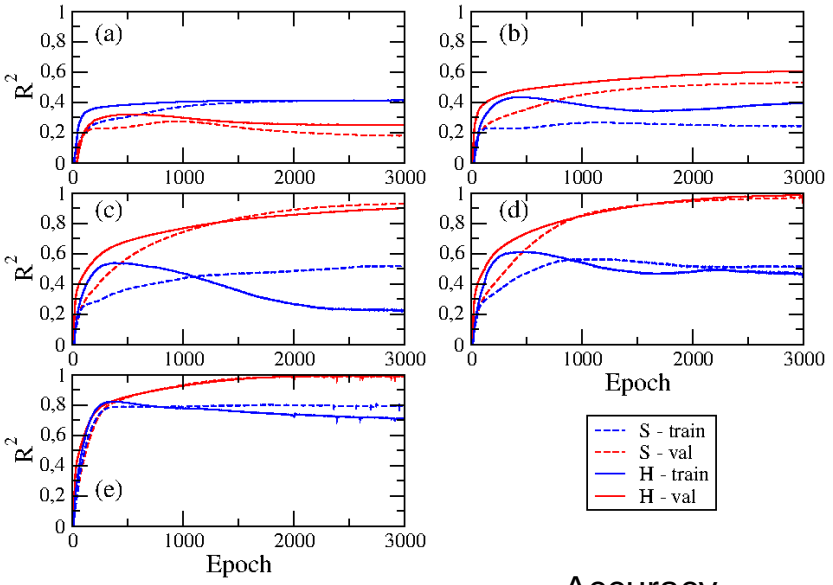
Pachete software: TensorFlow + Keras, PyTorch, Scikit-learn

Caracteristici:

- **TensorFlow 2.2 + Keras**: Implementare retele neurale (standard, convolutive etc); limbaj Python3, paralelism prin fire de execute (threading), calcul distribuit pe GPU, masini/HPC, TPU multiple (in lucru).
- **PyTorch**: similar cu TF, cu capacitate de calcul distribuit
- **Scikit-learn**: implementeaza diferite metode de tip ML, e.g. suport vector machines, random forests, dar si de pre-procesare a setului de date initial (dimensionality reduction).



Loss function



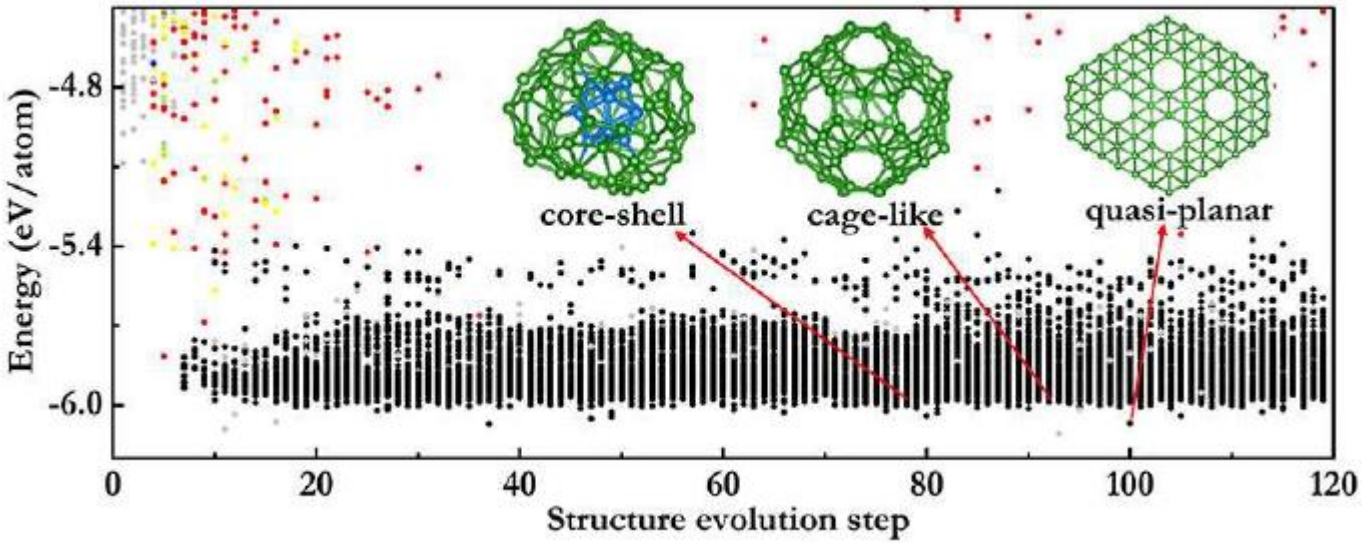
Accuracy

Algoritmi evolutivi

Pachet software: CALYPSO

Caracteristici:

- Implementeaza algoritm de tip Particle Swarm Optimization (PSO)
- Instantele sunt calculate cu DFT, dinamica moleculara
- se pot optimiza materiale (structura cristalina + compozitie) pentru diferite proprietati fizice (gap electronic, duritate)
- capacitate de calcul distribuit



Exemplu: cluster B84

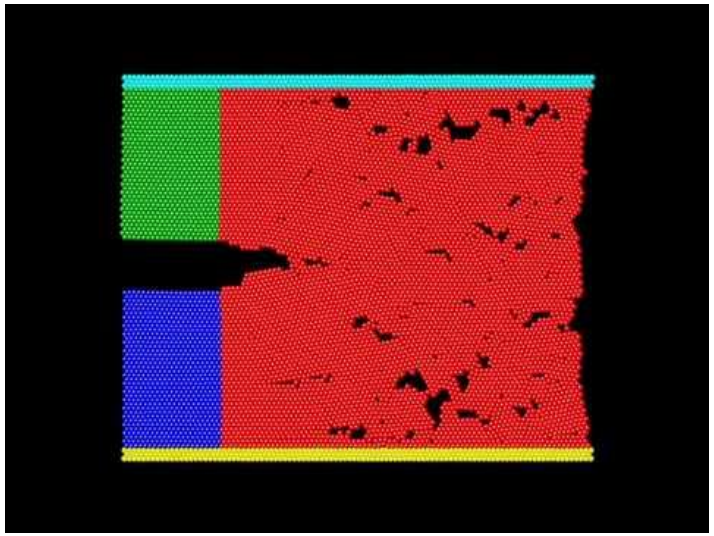
Tong et al., Faraday Discuss. 211, 31 (2018)

Dinamica moleculara

Pachet software: LAMMPS

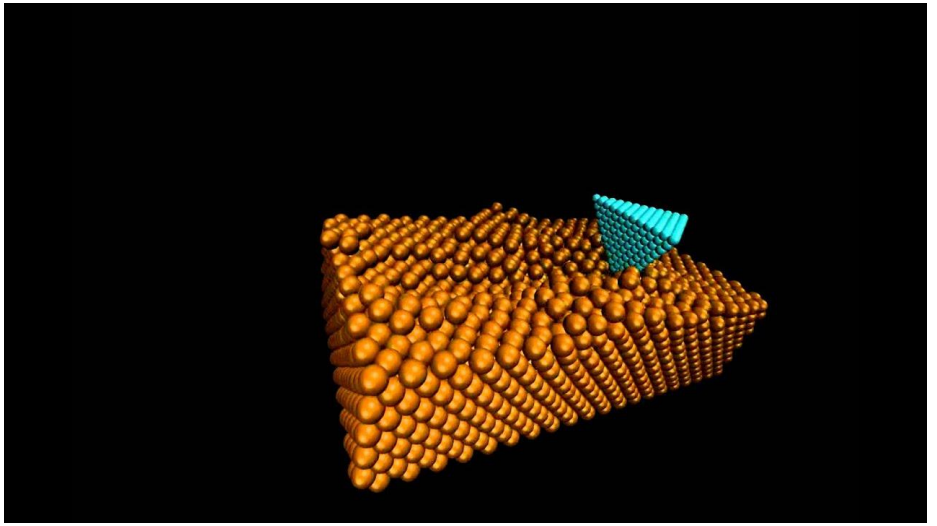
Caracteristici:

- Implementeaza dinamica moleculara cu camp de forte parametrizat
- Million to Billion atoms https://lammps.sandia.gov/bench.html
  *Lenard-Jones benchmark on Cray XT3: 40 billion atoms, 10000 cores, 979.0 s, parallel efficiency=96.0%,2.59 Tflop (2006)
- Aplicatii: transport de ioni in materiale perovskitice, nanoindentare
- Implementare MPI, GPU



Exemplu: crack formation

https://www.youtube.com/watch?v=GTJ_FOrjDiY



Exemplu: nanoindentation

https://www.youtube.com/watch?v=xsUREltXiyw

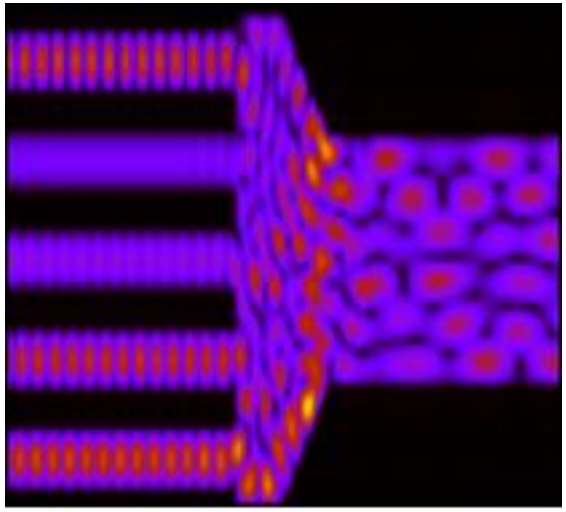
Dispozitive cuantice neurale

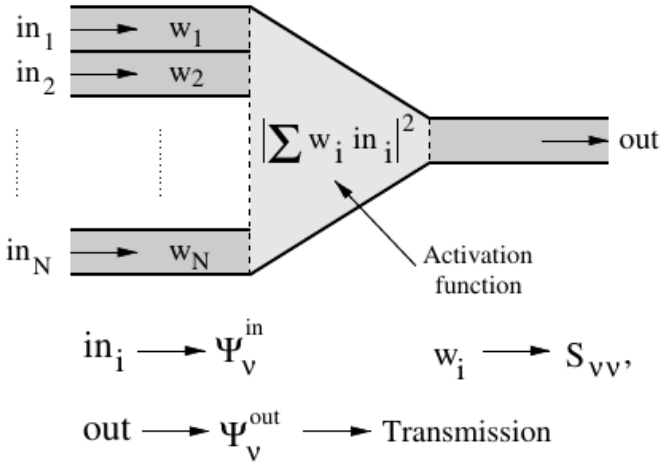
Metodologie: Formalism de imprastiere (metoda matricii R) pentru simularea unui neuron cuantic

Pachete software: Cod dezvoltat in-house, **C/MPI, LAPACK, SCALAPACK**

Modelul de neuron balistic este echivalent un un neuron McCulloch-Pitts in cazul unui sistem *single-mode.*

Extinderea modelului in cazul unui sistem de tip *multi-channel*, *bi-particula*.





G.A. Nemnes et al., Physica Stat. Sol. A 1900936 (2020)

Sumar

1. Se vor realiza servicii si aplicatii informatice pentru modelarea proprietatilor fizice in nanostructuri. Instalare, testare, realizare benchmarks pentru librarii specifice.

2. Implementare scheme de tip high through-put pentru calcule DFT si de dinamica moleculara. Rezultatele servesc pentru 3 (a) si 3 (b).

3. a). Implementare tehnici de tip machine learning (retele neurale artificiale) pentru screening proprietati de material.
b). Implementare modele evolutive pentru optimizarea proprietatilor de material, prin identificarea de noi faze structurale.

4. Generalizarea schemei de calcul pentru implementarea formalismului de imprastire. Modelare nanodispozitive cuantice neurale. Explorarea unor noi concepte de calcul in sisteme neuromorfice.