Analysis the Structures of Aluminas using DFT and Artificial Intelligence

[1,2*]Christian Rodriguez, [2,3]Xim Bokhimi
[1]Center of Research in Applied Science and Advanced Technology, National Polytechnic Institute
[2]Physics Institute, [3]DGAPA, National Autonomous University of Mexico
*e-mail: chrodriguez@estudientes.fisica.unam.mx

ABSTRACT

Creating a methodology to generate potentials of Neural Network and with this calculate different properties for different alumina's phases and these can be comparable with the reference calculations of DFT, the prediction of geometries, energies, atomic forces and atomic charges, at a lower computational cost, with a greater number of atoms and at longer Molecular Dynamics (MD) calculations, which resemble what happens in the laboratory.

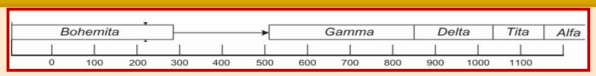
INTRODUCTION

The alumina's has been studied as they are widely used around of 45,000 ton/year[1] by his physical and chemical properties. The computational calculations will allow us to generate information about the crystalline structure to help explain the behavior and to improve the research in the development of nanomaterials based on it

DFT calculations
- Solid state technique (super cell)
- <500 atoms
- High computational cost
- Simulation times = Picoseconds
- Infrastructure limitations

Artificial Intelligence Algorithm
- Large clusters> 100,000 atoms
- Simulation times> nanoseconds
- Actual laboratory sizes
- Precise = DFT
- Few CPU's or / and GPU's

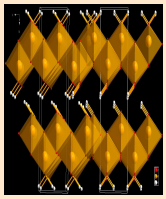
TRANSITION PHASES OF ALUMINAS

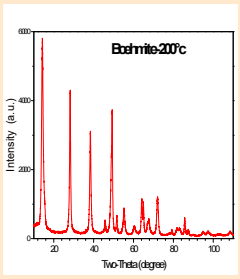


Crystallographic	Boehmite	Gamma-Alumina (Structures Models $Mg^{IV}[Al^{VI}_2]O_4$) [2,3]		Alpha-Alumina
Symmetry	Orthorhombic	Cubic	Tetragonal	Hexagonal
Space Group	Cmcm (63)	Fd-3m (227)	I41/amd (141)	R -3 c (167)
Parameters	a=2.8691Å b=12.2336Å c=3.6923Å	a=7.911Å	a=5.652Å b=7.871Å	a=4.7540Å c=12.9820Å

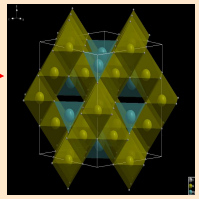
Boehmite synthesis was obtained by hydrothermal process , the γ-alumina and α-alumina was obtained by calcination, the lamellar crystals of the boehmite was transformed by dehydroxylation into γ-alumina with structures models of spinel[2,3] and with a considerable of stacking faults defects, to the final phase more crystalline α-alumina.

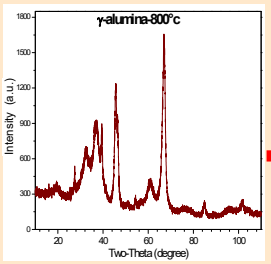
Boehmite AlO(OH) (Precursor)



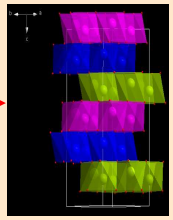


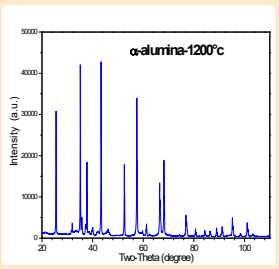
Gamma-Alumina γ-Al_2O_3 (Metastable structure)





Alpha-Alumina α-Al_2O_3 (Stable structure)

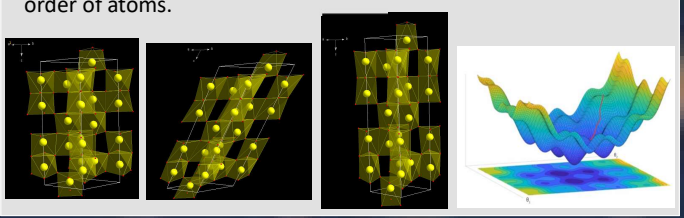




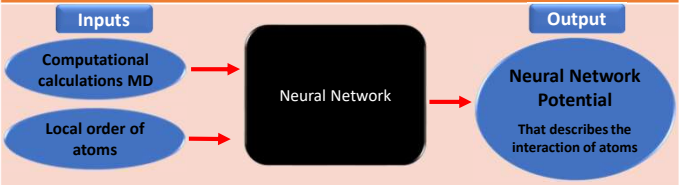
DFT CALCULATIONS

The DFT calculation was performed with the method of Molecular Dynamics with the initial atomic distribution of the crystallography of α-Alumina at different temperatures and arrangements, generating many of potential surface-energy (PES) points, that will feed to an algorithm of "Machine Learning", give the local order of atoms.

CONDITIONS	
Crystallography	α-Alumina
Cluster	< 200 Atoms
Program	CP2K
Job Type	Molecular Dynamics
Method	DFT
Functional	PBE
Basis set	DZVP-MOLOPT



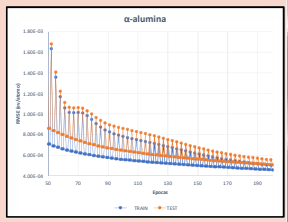
ARTIFICIAL INTELLIGENGE ALGORITHM



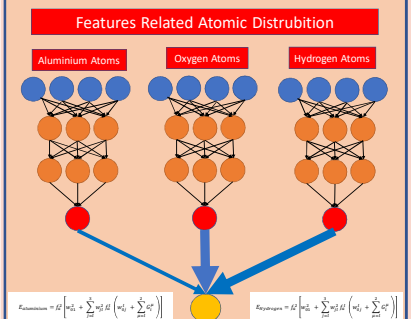
POTENTIAL ENERGY SURFACE USING ARTIFICIAL INTELLIGENCE

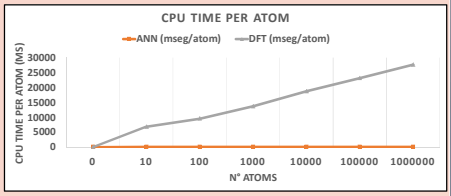
The potential of ANN was generated with which systems of up to millions of atoms can be calculated, with the same precision as the calculations of first principles with a calculation time of 4 smaller orders.

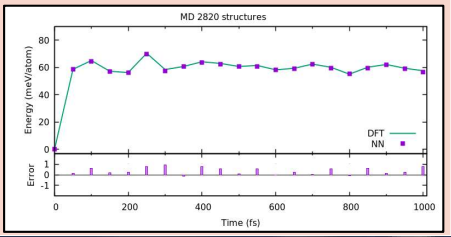
Plataform	Aenet, ASE, CP2K
Metric	RMSE
Optimization	Levenger-Marquardt
Samples	2820
Epoch's	200
GPU	Nvidia-GeForce
Execute Time	50 hrs



NEURAL NETWORK ARCHITECTURE 130-10-10-1







PRELIMINARY RESULTS

The NN potential of α-alumina was constructed. It has been shown that the reference energies can be reproduced very accurately not only for the structures included in the training set but also for the independent test set. In later stages, the information of the other phases will be used to obtain a potential of all the aluminas and can contribute to the knowledge of the structure of γ-alumina.

REFERENCES

[1] Knozinger, Ratsamay, P. Catal, Rev –Sct , Eng 1987, 17, 31.
[2] Tsybulya, N. Kryukova, Physical Review B77, 024112, 2008
[3] Pakharukova, Tsybulya, Juornal Solid Chesmistry, 246, 284, 2017.