



INFORMAȚII PERSONALE Chihaiia Viorel

vchihaia@icf.ro

LOCUL DE MUNCĂ

Institutul de Chimie Fizica Ilie Murgulescu, Academia Romana, Bucuresti, Romania.

EXPERIENȚA PROFESIONALĂ

2000, Post-doctorat Universitatea Keimyung, Taegu, Coreea
2001-2004, Post-doctorat Universitatea Goettingen, Germania
2010, Cercetator invitat, Institutul de Stiinta Atomica si Moleculara, Academia Sinica
2011-2015, Cercetator, Jülich Supercomputing Centre, Germania

1990 - până astăzi

Cercetator Stiintific II

Laboratorul de Chimia Suprafetei si Cataliza, Institutul de Chimie Fizica Ilie Murgulescu

Sectorul de activitate Simulare asistata de calculator in stiinta materialelor

EDUCAȚIE ȘI FORMARE

1989, Diploma, "Semiempirical Calculation Methods of MO. Applications for AB₂ AB₃ and AB₄ Molecules", Universitatea Bucuresti

1999, Doctorat "Simulation at Atomic Scale of Surface Processes. Hydrogen Interaction with MgO(001) Surface", Institutul de Chimie Fizica Ilie Murgulescu,

COMPETENTE PERSONALE

Structura electronica a sistemelor moleculare si a solidului

Proprietati si fenomene ale suprafetelor, interfetelor si cataliza

Simulari Dinamica Moleculara si Monte Carlo

Simulari la scala atomica, nano- si meso-scala

Programare seriala si paralela
Constructie si administrare clustere HPC

Limba(i) maternă(e) Romana

Competențe de comunicare

- bune competențe de comunicare dobândite prin experiența proprie de cercetator

Competențe organizaționale/manageriale

- bun co-echipier (am facut parte din mai mult de 20 proiecte de cercetare)
- leadership (am fost director pentru 8 proiecte nationale si internationale)

Competențe dobândite la locul de muncă

- Cunostinte avansate de metode de structura electronica in chimie si fizica starii solide
- Constructia si administrarea de clustere de tip High Performance Computing

Publicații	
44 articole ISI	NTX Huynh, OM Na, V Chihaiia, A computational approach towards understanding hydrogen gas adsorption in Co-MIL-88A, RSC Advances, 7 (2017) 39583. D. N. Son, O. K. Le, M. T. Hiep and V. Chihaiia, Magnetic anisotropy of ultrathin Pd ₄ Co (111) film by first-principles calculations, J. Sci.: Adv. Mat. Dev., 3 (2018) 243. H. S. AlMatrouk, V. Chihaiia and V. Alexiev,

Density functional study of the thermodynamic properties and phase diagram of the magnesium hydride,
Calphad, 60 (2018) 7.

N. Th. X. Huynh, V. Chihaiia and D. N. Son,
Hydrogen storage in MIL-88 series,
J. Mater. Sci., 54 (2019) 3994.

N. Th. X. Huynh, V. Chihaiia and D. N. Son,
Enhancing hydrogen storage by metal substitution in MIL-88A metalorganic Framework,
Adsorption, 26 (2020) 509.

Ong Kim Le, Viorel Chihaiia, My-Phuong Pham-Ho and Do Ngoc Son,
Electronic and optical properties of monolayer MoS₂ under the influence of polyethyleneimine adsorption and pressure,
RSC Adv., 2020, 10, 4201-4210

H. S. AlMatrouk, F. Al-Ajmi, D. N. Son, V. Chihaiia and V. Alexiev,
The Pressure-Temperature Phase Diagram Assessment for Magnesium Hydride Formation/Decomposition Based on DFT and CALPHAD Calculations,
Mod. App. Matrl. Sci., 4 (2021) 467.

R.M. Visan, A.R. Leonties, L. Aricov, V. Chihaiia and D.G. Angelescu,
Polymorphism of chitosan-based networks stabilized by phytate investigated by molecular dynamics simulations,
PCCP, 23, 2021, 22601-22612

TT Pham, TN Pham, V Chihaiia, QA Vu, TT. Trinh, TT Pham, LV Thang si NG Do,
How do the doping concentrations of N and B in graphene modify the water adsorption?,
RSC Adv., 2021, 11, 1956

V. K. Dien, O. K. Le, V. Chihaiia, M. P. Pham-Ho, N. G. Do,
Monolayer transition-metal dichalcogenides with polyethyleneimine adsorption,
J. Comput. Electron., 20, 2021, 135–150

O. K. Le, V. Chihaiia, V. V. Ond si N. G. Do,
N-type and p-type molecular doping on monolayer MoS₂,
RSC Adv., 2021, 11, 8033

R. Bucuresteanu, L. M. Ditu, M. Ionita, I. Calinescu, V. Raditoiu, B. Cojocaru, L. O. Cinteza, C. Curutiu, A. M. Holban, M. Enachescu, L. B. Enache, G. Mustatea, V. Chihaiia, A. Nicolaev, EL Borcan and G Mihaescu,
Preliminary Study on Light-Activated Antimicrobial Agents as Photocatalytic Method for Protection of Surfaces with Increased Risk of Infections,
Materials 2021, 14, 5307.

H. S. AlMatrouk, F. Al-Ajmi, N. G. Do, V. Chihaiia and V. Alexiev,
The Pressure-Temperature Phase Diagram Assessment for Magnesium Hydride Formation/Decomposition Based on DFT and CALPHAD Calculations, Mod App Matrl Sci.4 (2021)

N. G. Do, V. Chihaiia and P. T. Thi, Mechanism of Oxygen Reduction Reaction on Monolayer WTe₂ with and without S Dopant at Low Coverage, e-Journal of Surface Science and Nanotechnology 19, 119–124 (2021)

	<p>Phan Thi Hong Hoa, Viorel Chihaiia, Ong Kim Le, Pham Thanh Hai, Dang Long Quan, Huynh Tat Thanha and Do Ngoc Son Selectivity of volatile organic compounds on the surface of zinc oxide nanosheets for gas sensors Phys. Chem. Chem. Phys., 2022, 24, 20491–20505</p> <p>Viorel Chihaiia, Mihalache Ghinea, Stefan Chihaiia and Andreea Neacsu Mathematical Chemistry Approaches for Computer-Aid Design of Free-Shaped Structures in Architecture and Construction Engineering Mathematics 2022, 10, 4415</p> <p>Insights into Interaction of CO₂ with N And B-Doped Graphenes Nguyen Thi Xuan Huynh, Viorel Chihaiia And Do Ngoc Son Communications in Physics, 2022, 32, 243-252</p> <p>Razvan Bucuresteanu, Monica Ionita, Viorel Chihaiia, Anton Ficai, Roxana-Doina Trusca, Cornelia-Ioana Ilie, Andrei Kuncser, Alina-Maria Holban, Grigore Mihaescu, Gabriela Petcu, Adela Nicolaev Ruxandra M. Costescu, Mihai Husch, Viorica Parvulescu and Lia-Mara Ditu Antimicrobial Properties of TiO₂ Microparticles Coated with Ca- and Cu-Based Composite Layers Int. J. Mol. Sci. 2022, 23, 6888</p> <p>Ong Kim Le, Viorel Chihaiia, Phan Thi Hong Hoa, Pham Thanh Hai and Do Ngoc Son Physical insights into the Au growth on the surface of a LaAlO₃/SrTiO₃ heterointerface RSC Adv., 2022,12, 24146-24155</p> <p>Nguyen Thi Xuan Huynh, Ong Kim Le, Tran Phuong Dung, Viorel Chihaiia and Do Ngoc Son Theoretical investigation of CO₂ capture in the MIL-88 series: effects of organic linker modification RSC Adv., 2023,13, 15606-15615</p> <p>Tran Phuong Dung, Viorel Chihaiia and Do Ngoc Son Effects of functional groups in iron porphyrin on the mechanism and activity of oxygen reduction reaction RSC Adv., 2023,13, 8523-8534</p> <p>Ong Kim Le, Viorel Chihaiia, Do Ngoc Son Effects of N-doped concentration in graphene on CO₂ adsorption Science & Technology Development Journal - Engineering and Technology, 2023, 6, 1809-1816</p>
<p>Director Proiecte</p>	<p>“Cadru combinat experimental - calcule numerice pentru studiul stocarii hidrogenului in nanoparticule bazate pe magneziu”, Proiect nr. 302PED2020.</p> <p>"Molecular simulations for penetrable fluids confined in nanopore systems", Program Capacities/Module III ANCS, Bilateral cooperation Romania-Corea 462/18.02.2011</p> <p>"New complex hydrides for hydrogen storage in adequate reservoir for vehicle applications" (Romanian) National Center for Programs Management, Grant STOHICO 72-196/2008,</p> <p>"Virtual Group for Atomic Scale Simulations in Materials Science", ANCS Research Grant , Capacities Project 84 CpI/13.09.2007</p>
<p>Prezentări invitate 2001-2023</p>	<p>Computer Modeling of Materials and Radiation, Viorel Chihaiia, Invited seminar, CETAL - National Institute for Laser, Plasma & Radiation Physics, 9 May 2018</p> <p>Investigation of Irradiation Effects on the Structural Properties of Cellulose, Viorel Chihaiia,</p>

	<p>Invited seminar, IRASM - Horia Hulubei National Institute of Physics and Nuclear, Engineering, Magurele, 18th July 2018</p> <p>“Research and Support Activities of the Simulation Lab Molecular Systems”, Viorel Chihaiia, Invited lecture, International Conference on Computational Science and Engineering, Ho Chi Minh, City, Vietnam, August 21 - 23, 2014</p> <p>“Short Survey of Computer Simulations for Energy Materials”, V. Chihaiia, Th. Müller and G. Sutmann, JSC–IEK - Workshop, 17 July 2013, Jülich, Germany</p> <p>“The DFT study of the gold clusters adsorbed on the surface MgO(001)”, Institute of Atomic and Molecular Science, Sinica Academy, Taipei, Taiwan, 2 July 2010</p> <p>“Numerical Simulations in Material Science”, IBM High Performance Scientific Computing Workshop, University Politehnica of Bucharest, Romania, June 14-18 2010</p> <p>www.hpc-icf.ro – Grup Virtual de Simulare la Scala Atomica in Studiul Materiei, Romanian Academy, 28 April 2009</p> <p>“Atomic Scale Simulation in Material Science”, V. Chihaiia, UPB GridInitiative 2008 - High Performance Computing Applications, Bucharest, 23 July 2008</p> <p>“Molecular Dynamics Study for the Adsorption of the Small Molecules on the Deformed Nanotubes”, The 3rd Polymer Gel Research Cluster Center, Yeungnam University, Korea, 13-14 April 2007</p> <p>“Divergence-Free Algorithm for the Rigid-Body Rotation Based on the Propagation of the Body Orientation”, V. Chihaiia, S.-H. Suh And G. Sutmann</p> <p>Invited seminar to “John von Neumann Institut for Computing”, Juelich, Germany, 10th October 2006,</p> <p>“A Growth Mechanism for Clathrates. Combined Semiempirical Hartree-Fock and Density Functional Theory Studies.“ Viorel Chihaiia, Tzonka Mineeva, Valentin Alexeev and Soong-Hyuck Suh, Invited lecture to “Third Humboldt Conference on Computational Chemistry” , June 24-28, 2006, Varna, Bulgaria</p> <p>“Atomic Scale Modelling in Material Science”, Invited seminar Faculty of Environmental and Chemical Enegeneering, Seonam University, Seonam, South Korea, 14 September 2000.</p> <p>“Magnesium Oxide. Bulk and Surface Properties”, Invited seminar to Chemical Enegeneering Faculty, Keimyung University, Taegu, South Korea, 21 July 2000</p>
Conferințe	<p>“ZnO Nanostructures for Gas Sensing” Aurelian Marcu, Razvan Mihalcea, C. Samoil, E. Slushanschi, V.Chihaiia, I. Nicolae and C.Viespe, SNAIA, 8-11 December 2020, École Nationale Supérieure de Chimie de Paris, 11, Rue Pierre et Marie Curie, Paris, France Smart NanoMaterials 2020 - Advances, Innovation and Applications - https://snaia.eu/</p> <p>POSTER: Investigation of Irradiation Effects on the Structural Properties of Cellulose by Molecular Dynamics Simulations Viorel Chihaiia, Ioan Valentin Moise and Ioana Stanculescu ChemCH2018 – 5th International Congress on Chemistry for Cultural Heritage Bucharest, Romania, 3rd-7th July, 2018</p>

PRESENTATION: Theoretical Study of the Magnesium Hydride Decomposition
H. S. AlMatrouk, V. Alexiev and V. Chihaiia,
European Hydrogen Energy Conference 2018 Malaga, Spain. 14-16th March, 2018

POSTER: ReaxFF Molecular Dynamics Investigation on the Magnesium Hydride Fracture
Hasan S. AlMatrouk, Viorel Chihaiia, and Valentin Alexiev
Energy7, Manchester, UK
13-17 August 2017

PRESENTATION: Computational investigation of pressure and temperature effects on the structural stability of Mg-H system using the quasi-harmonic model calculations
Hasan S. AlMatrouk, Viorel Chihaiia and Valentin Alexiev
21st World Hydrogen Energy Conference 2016. Zaragoza, Spain.
13-16th June, 2016

Recent Research and Support Activities of the Simulation Lab Molecular Systems
Lectures at the 46th IFF Spring School - Functional Soft Matter
4th March 2015, Jülich, Germany
Multiscale Coupling Methods. MD-FEM in IBIsCO code
Viorel Chihaiia
Division Seminar, Jülich Supercomputing Centre, Jülich, Germany
13rd May 2014

Oxygen Reduction Reactivity of PdCo Alloy upon Co Content
Do Ngoc Son, Ong Kim Le, Viorel Chihaiia, Kaito Takahashi
Oral presentation, 39th National Conference on Theoretical Physics, Center for Theoretical Physics & Center for Computational Physics, Buon Ma Thuot, Vietnam
28-31 July 2014

Surface Oxide Formation on Pt Cathode of Proton Exchange Membrane Fuel Cells: Effects of Reaction Intermediates
Do Ngoc Son, Nguyen Thi Gam, Kaito Takahashi, Viorel Chihaiia
Poster, 39th National Conference on Theoretical Physics, Center for Theoretical Physics & Center for Computational Physics, Buon Ma Thuot, Vietnam
28-31 July 2014

Co Content Effect on Oxygen Reduction Reaction Activity of PdCo Catalyst, Do Ngoc Son, Ong Kim Le, Viorel Chihaiia, Kaito Takahashi
Poster, International Conference on Computational Science and Engineering, Ho Chi Minh City, Vietnam,
August 21 - 23, 2014

SimLab Molecular Systems
Chihaiia, V.; Halver, R.; Müller, Th.; Schiller, A.; Sutmann, G.
Poster, NIC Symposium 2012, Jülich, Germany, 07.02.2012 - 08.02.2012
D36/003/06 Working Group Meeting, Sibiu, ROMANIA
21-22 May 2010

Semiempirical Study of Reactivity of Small Gold Clusters Deposited on the MgO(001) surface
V. Chihaiia, G. Munteanu and V. Alexiev
COST D36/003/06 Working Group Meeting, Institute of Nanostructured Materials, CNR, Palermo
15-16 May 2009

“Effects on catalytic activity of structure and dynamic properties of liquids confined in silica mesopores with hexagonal array”
V. Chihaiia, V. Parvulescu, S.-S. Han, J.-Y. Bae, S.-H. Suh
14th INTERNATIONAL CONGRESS ON CATALYSIS, Seoul, Korea,
13 – 18 July 2008

“Formation of metallic clusters on MgO(001) surface. An atomic scale study” V. Chihaiia and G. Munteanu
COST D36/003/06 Working Group Meeting, Nice, France
12 Oct 2008
Atomistic simulations of the gold clusters adsorbed on the surface MgO(001) V. Chihaiia, G. Munteanu and V. Alexiev
COST D36/003/06 Working Group Meeting, Sibiu, ROMANIA
21-22 May 2010

Semiempirical Study of Reactivity of Small Gold Clusters Deposited on the MgO(001) surface
V. Chihaiia, G. Munteanu and V. Alexiev
COST D36/003/06 Working Group Meeting, Institute of Nanostructured Materials, CNR, Palermo
15-16 May 2009

“Effects on catalytic activity of structure and dynamic properties of liquids confined in silica mesopores with hexagonal array”
V. Chihaiia, V. Parvulescu, S.-S. Han, J.-Y. Bae, S.-H. Suh
14th INTERNATIONAL CONGRESS ON CATALYSIS, Seoul, Korea,
13 – 18 July 2008

“Formation of metallic clusters on MgO(001) surface. An atomic scale study” V. Chihaiia and G. Munteanu
COST D36/003/06 Working Group Meeting, Nice, France
12 Oct 2008

“Molecular dynamics study for the adsorption of small molecules on deformed nanotubes”, V. Chihaiia, I. Sitaru, A. Ghita, B.-S. Seong and S.-H. Suh
The 3rd Korea/Romania Joint Workshop: Molecular Science and Engineering, Keimyung University, Korea, April 27, 2007

“The axis-rotation formula and some of its application to Computational Chemistry”, S.-H. Suh, C.-S. Lee, V. Chihaiia and G. Sutmann
“Third Humboldt Conference on Computational Chemistry”, Varna, Bulgaria, June 24-28, 2006

“Theoretical Study of Growth Mechanism of Clathrates” V. Chihaiia and S.H. Suh
2nd Korean-Romanian Workshop on Molecular Science and Engineering, Bucharest, ROMANIA, September 8, 2006

“Water molecule adsorption on the clean and Sn doped γ -alumina surface”
V. Chihaiia, M. Caldararu, C. Munteanu, C. Hornoiu, M. Carata, K. Sohlberg, S.H. Suh
The International Conference of Physical Chemistry ROMPHYSICHEM-12, Bucharest, ROMANIA, September 6-8, 2006

“The clathrate growth by the Coalescence of the small buckyball clusters” Viorel Chihaiia, Chang-Sup Lee and Soong-Hyuck Suh
“The 1st Korean-Romanian Workshop”, Romania Academy, Bucharest, 2005

	<p>“The Stability of the Small Buckyballs and Their Coalescence” Viorel Chihaiia, Chang-Sup Lee and Soong-Hyuck Suh, Zilele Academice Timisorene, Timisoara, Romania, 26-27 May 2005.</p> <p>“Structure of Methane Clathrate Hydrate Surface (001) by Molecular Dynamics Simulations” V. Chihaiia, St. Adams and W.F. Kuhs N2-M2 Neutrons and Numerical Methods 2, Institute Laue Langevin, Grenoble, France, 15-18 September 2004.</p> <p>“Electronic Band Properties of the Ice Ih and II”, V. Chihaiia, St. Adams and W.F. Kuhs Electronic Band Structure Workshop, Aachen, Germany, 8-10 February 2004.</p> <p>“Computer Simulation of Proton Rearrangements in 512 and 51262 Buckyball Water Clusters. Influence on the DOS”, V. Chihaiia, St. Adams and W.F. Kuhs Gordon Research Conference, “Water and Aqueous Systems”, Boston, US 8-10 September 2002</p> <p>“Computer Simulation of Proton Rearrangements in 512 and 51262 Buckyball Water Clusters” V. Chihaiia, St. Adams and W.F. Kuhs, "Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms", Kerkrade, Netherlands 25 February - 1 March 2002.</p> <p>“The Spin Hamiltonian Effective Approach to the Vibronic Effects – Selected Cases” F. Cimpoesu, K. Hirao, N. Stanica and V. Chihaiia, 16th International Jahn-Teller Conference, Leuven, Belgium, 26 August - 1 September 2002.</p> <p>“The Stability of 512 and 51262 Buckyball Water Clusters as a Function of their Dipole Moments and their Relevance for Gas-Water Interactions at the Ice Surface”, V. Chihaiia, St. Adams and W.F. Kuhs “Réactivité à la surface de la Glace”, Porquerolles, France , 17-21 September 2001.</p>
Organizare Workshop	<p>Co-organizer of the Workshop “Computing Methods for Hydrogen Storage”, Institute of Catalysis, Sofia, Bulgaria, 18 October - 2 November 2018</p> <p>Co-organizer of the Workshop “Computing Methods for Hydrogen Storage”, Institute of Catalysis, Sofia, Bulgaria, 18 October - 2 November 2017</p> <p>Co-organizer of Romania/Korea Joint Workshop: Molecular Science and Engineering Held annually in Korea or Romania, between 2005-2012</p> <p>Co-organizer of COST D36/003/06 Working Group Meeting, Sibiu, 21-22 May 2010</p>
Patent	<p>Palade Petru, Comanescu Cezar Catalin, Guran Cornelia, Chihaiia Viorel, Coldea Ioan Dorian, Patent OSIM nr. 128919/2017, “Hydrogen storage materials based on mixtures of amides-hydrides-borohydrides”.</p>
Referent	<p>Chemistry Journal of Moldova Crystal Research and Technology Energy and Environmental Science Journal of Materials Chemistry Journal of Physical Chemistry Journal of Chemical Physics New Journal of Chemistry Physical Chemistry Chemical Physics Revue Roumaine de Chimie Soft Matter RSC Advances</p>

