ХАБАРОВСКИЙ ФЕДЕРАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ ЦЕНТР ДВО РАН

ВЫЧИСЛИТЕЛЬНЫЙ ЦЕНТР
ДАЛЬНЕВОСТОЧНОГО ОТДЕЛЕНИЯ
РОССИЙСКОЙ АКАДЕМИИ НАУК

Компьютерный дизайн 2D материалов для современной наноэлектроники: успехи и перспективы

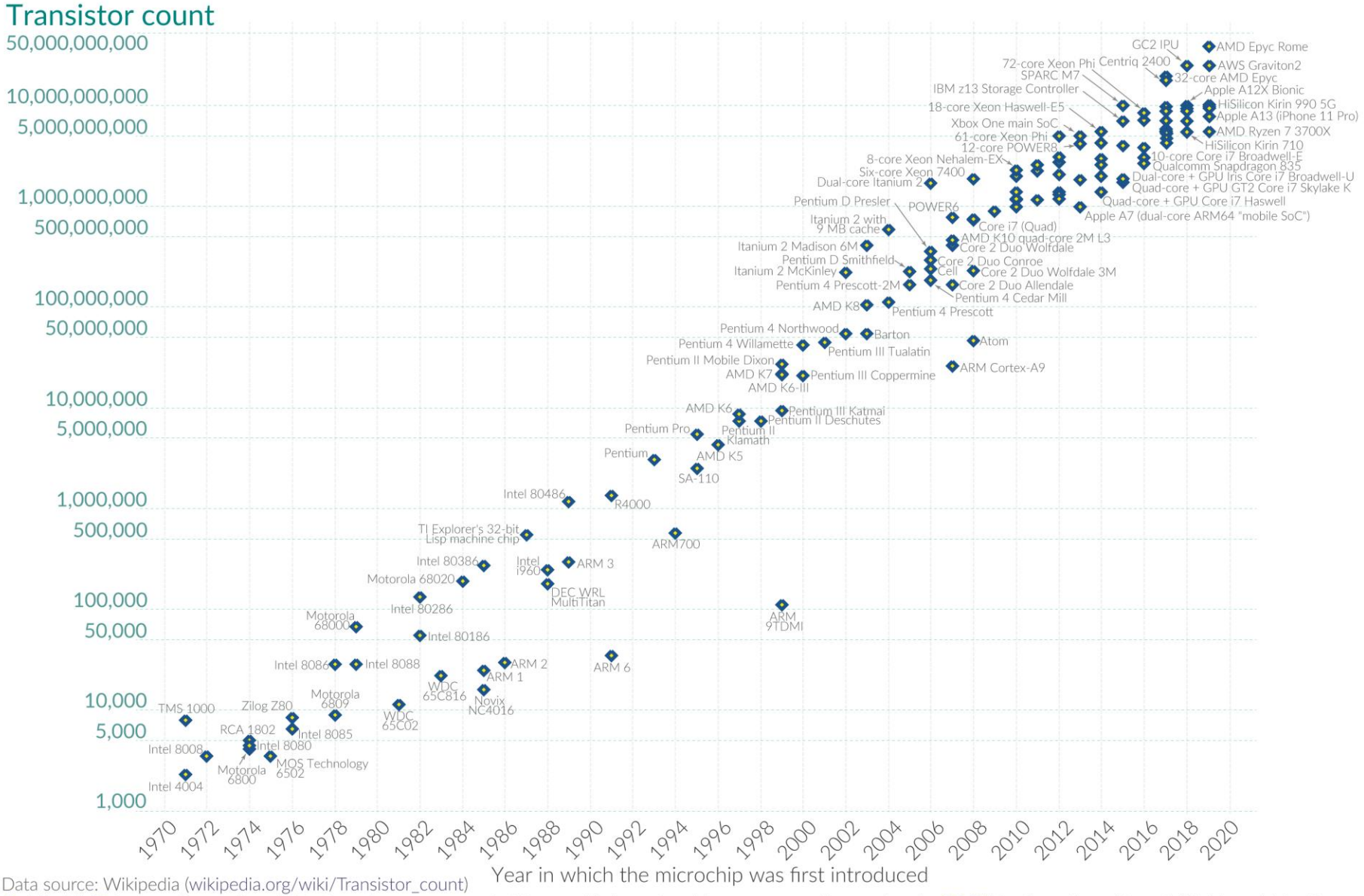
Andrey N. Chibisov,
PhD, Professor, Deputy Director for Research,
Computing Center of the Far Eastern Branch of the Russian Academy of Sciences, Leading Researcher
andreichibisov@yandex.ru
http://ru.linkedin.com/pub/andrey-chibisov/55/253/986/en

Introduction

Moore's Law: The number of transistors on microchips doubles every two years

Our World in Data

Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.



Data source: Wikipedia (wikipedia.org/wiki/Transistor_count)

Methods and approaches

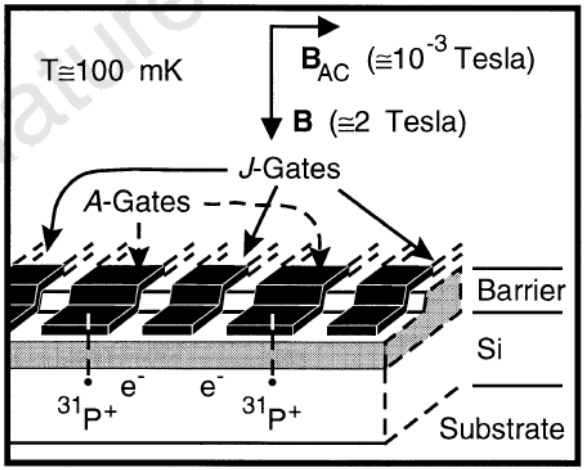
• Quantum Espresso, Vasp software package based on density functional theory and the pseudopotentials method.
• Perdew–Burke–Ernzerhof pseudopotentials for Si and P atoms in the generalized gradient approximation (GGA), noncollinear and spin-orbit coupling magnetization.
• Unit cell – 6×6×6 k–point
• 64 atoms supercell (P:Si) - 3×3×3 k–point
• Cut energy of plane waves 476.2 эВ
• Atomic relaxation –interatomic forces 0.026 эВ/Å.

Joint Supercomputer Center of the RAS (Moscow, Russia)

Shared Facility Centre 'Data Centre of FEB RAS' (Khabarovsk, Russia)

Major challenge:

The practical implementation of quantum computers



B.E. Kane. Nature. Vol. 393. 1998. P 133

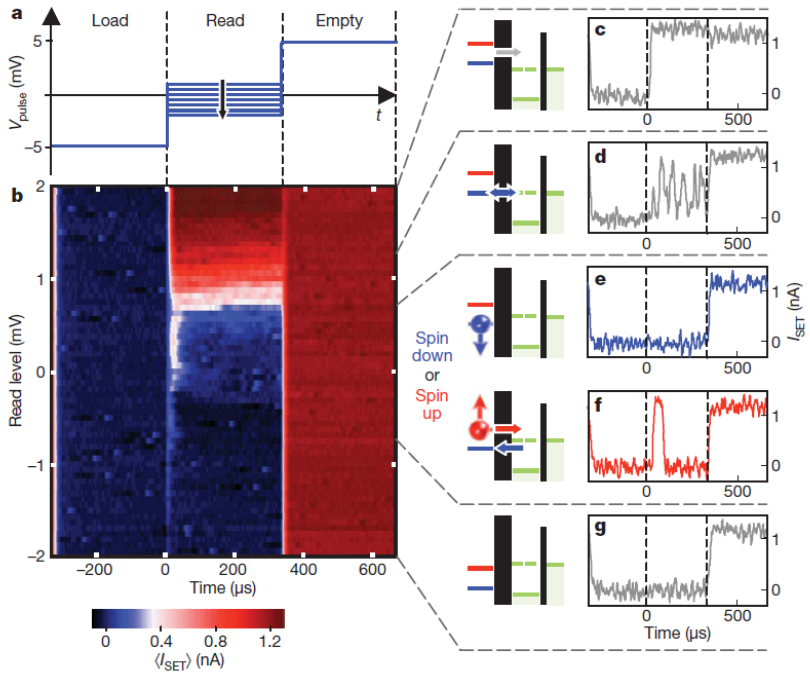
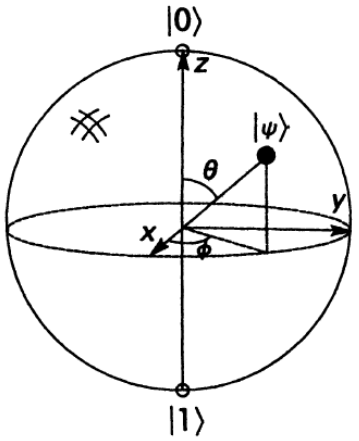


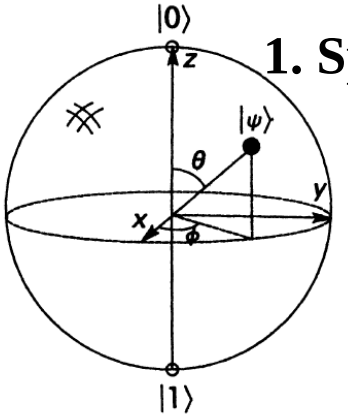
Figure 2 | Single-shot spin readout and calibration of the 'read' level. **a**, Three-level pulsing sequence for spin readout. The 'load' and 'empty' levels are kept constant, while the read level is scanned from high to low. **b**, SET current ⟨I_{SET}⟩, averaged over 128 single-shot traces (colour scale), as a function of the V_{pulse} level during the read phase. Data taken with an applied magnetic field $B = 5$ T and a detection bandwidth of 40 kHz (rise time ~10 μs). **c**–**g**, Examples of single-shot traces. **c**, Read level too high, $\mu_\downarrow > \mu_{SET}$: the electron always leaves the donor during the read pulse, regardless of its spin. **d**, $\mu_\downarrow \approx \mu_{SET}$: random telegraph signal indicates an electron switching between SET island and $|\downarrow\rangle$ state. **e**, **f**, Correct read level, $\mu_\downarrow < \mu_{SET} < \mu_\uparrow$: $I_{SET} = 0$ during the read phase indicates a $|\downarrow\rangle$ state (**e**). A single current pulse at the beginning of the read phase is the signature of a $|\uparrow\rangle$ state (**f**). The regime of correct read level is recognizable by the isolated increase in ⟨I_{SET}⟩ in **b**. **g**, Read level too low, $\mu_\uparrow < \mu_{SET}$: the electron never leaves the donor during the read pulse.

Andrea Morello. Nature. Vol. 467. 2010. P. 687



Important tasks:

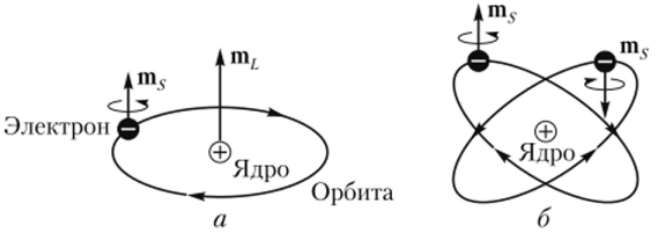
- **Investigate the Si atoms substitution by phosphorus.**
- **Calculate electronic properties.**
- **Investigate the P spins orientation.**



1. Spin orientation of the P atom excess electron

the most energetically favorable spin orientation
m_z=-1 (is the |1> quantum state in Bloch sphere)

(θ; φ) = 176°; 102°
- free atoms relaxation



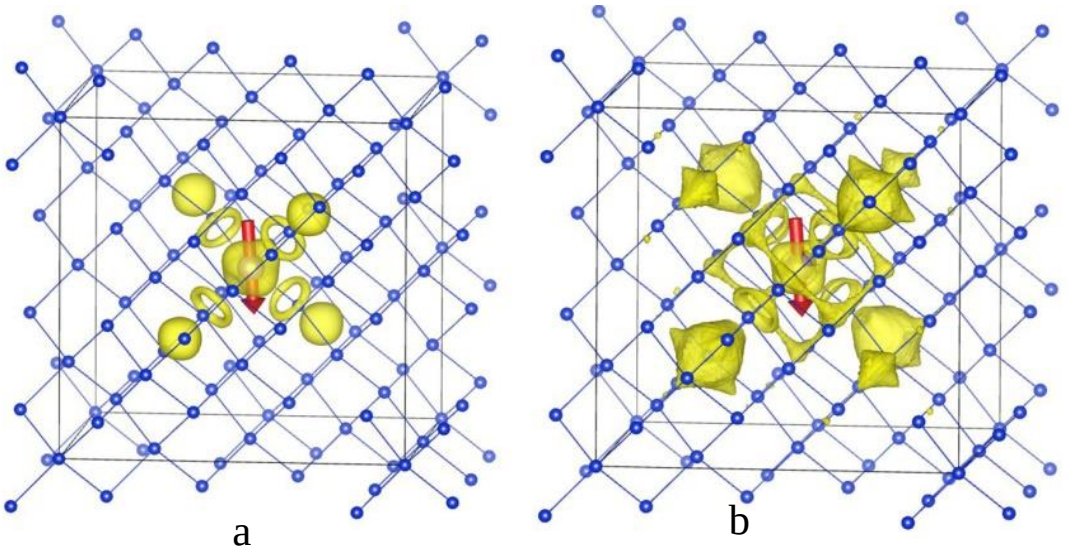
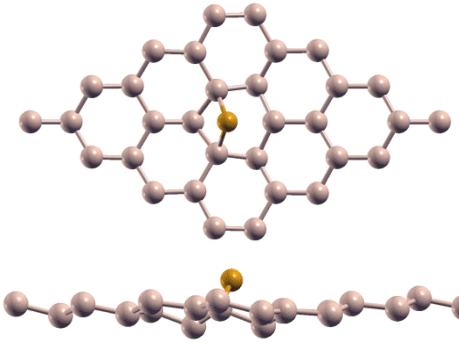


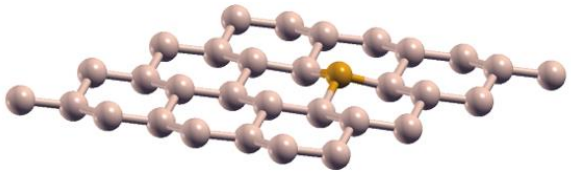
Fig. 1. a - the |1> spin orientation of the P atom and noncollinear magnetization **m**(**r**) (the $|\psi|^2$ electron localization density) of the P:Si atomic system; b - spin current density in the system.

Chibisov A.N., Chibisova M.A. ***Journal of Physical Chemistry Letters. 2020****. Vol. 11(11). P. 4427–4429 (****WoS Q1****, IF* 6.888*)*

2. Studies of the behavior of the phosphorus atom on the surface of silicene

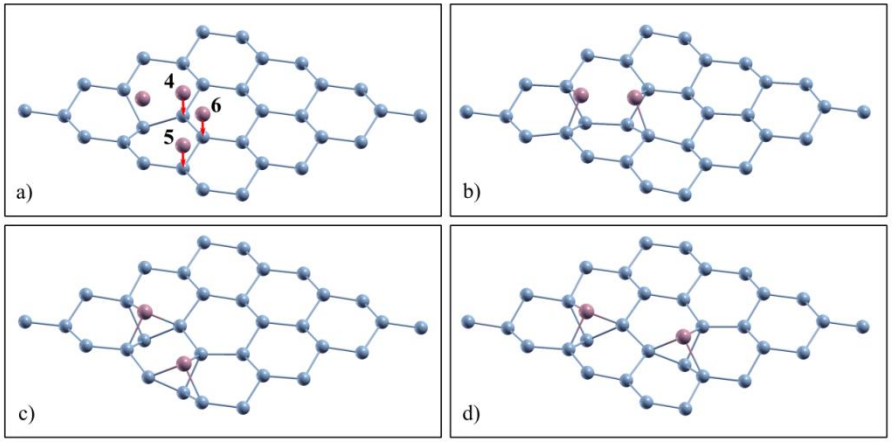


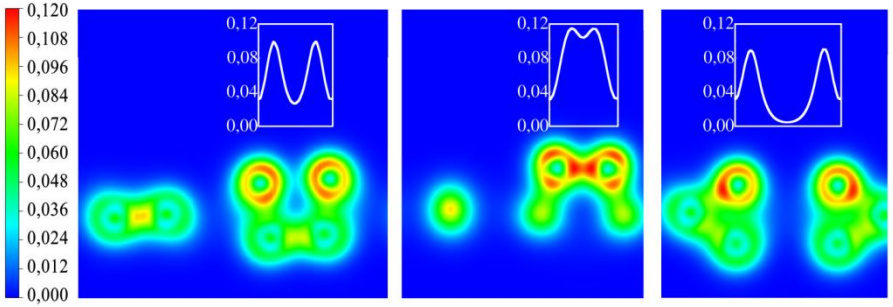
Phosphorus adsorption on silicene

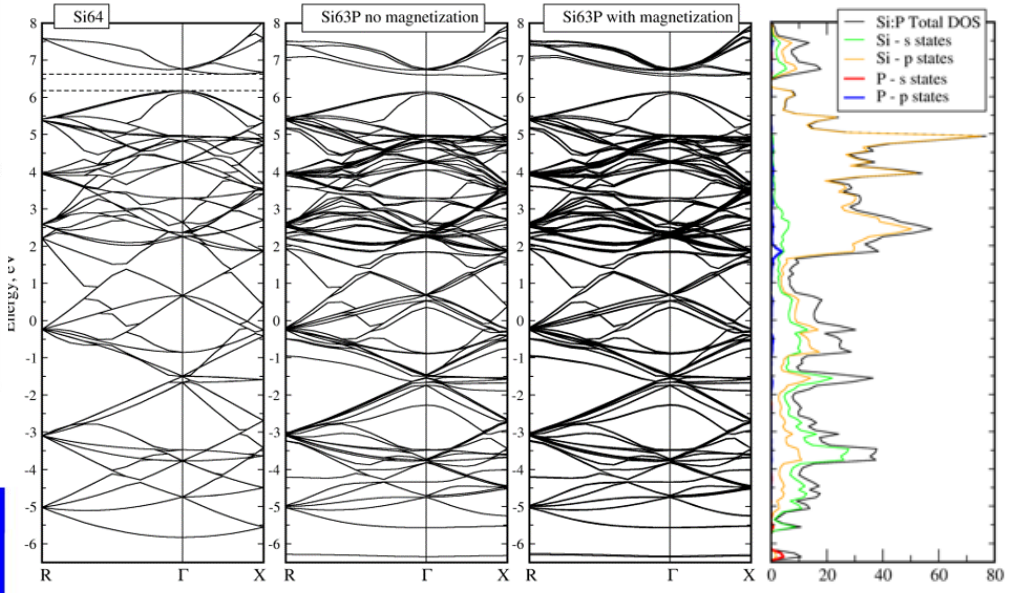


Silicon substitution by phosphorus in silicene (Si31P)

The energy gain of P adsorption compared to substitution is about 0.5 eV.

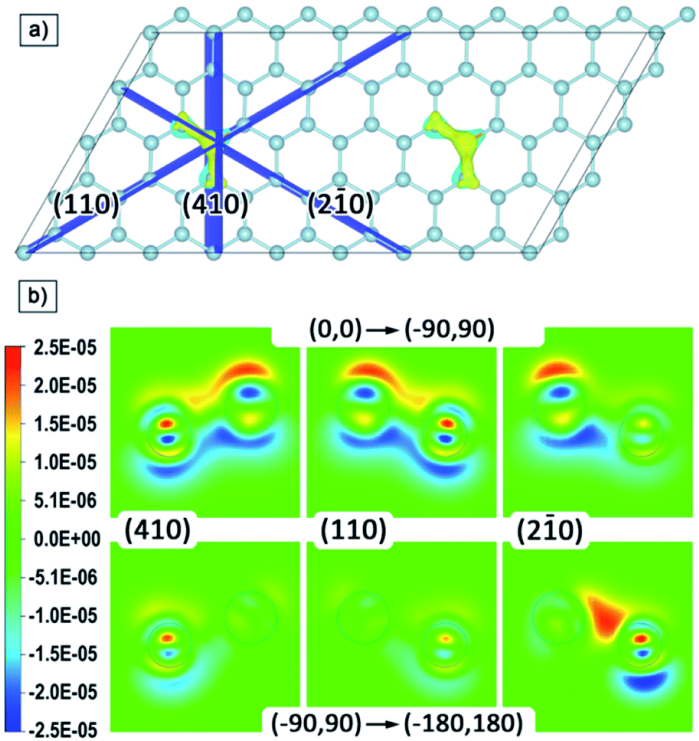






Band structures for pure silicon crystal (Si64) and for phosphorus-doped silicon (Si63P)

3 Design of numerical models for calculating quantum qubits.



The electronic and magnetic structure of phosphorus-doped silicene is calculated using the noncollinear density functional theory. It is found that the antiferromagnetic state for local magnetic moments of a pair of phosphorus atoms is preferable both in the presence and absence of magnetization. It is shown how the charge density changes in space in regions substituted by a phosphorus atom.

Atomic structure of the Si62P2 cell with planes passing through the phosphorus atom and its bonds with the nearest silicon atoms;

Gnidenko A.A., **Chibisov A.N., Chibisova M.A.**, Prokhorenko A.V. Quantum mechanical modelling of phosphorus qubits in silicene under constrained magnetization. // **RSC Advances.** 2021. 11. 33890-33894. https://doi.org/10.1039/D1RA05422H (**WoS Q2, SCOPUS Q1, IF 4.036**).

Chibisov A.N., Gnidenko A.A., **Chibisova M.A., Prokhorenko A.V.,** Yu Yang-Xin. Quantum-mechanical study of the optimal phosphorus atoms arrangement on silicene. // **Chemistry of Flat Materials**. 2023. Vol. 41. P. 100533 (**WoS Q2, SCOPUS Q1, IF 6.2**)

Results :

2020

Chibisov A.N., Chibisova M.A. ***Journal of Physical Chemistry Letters. 2020****. Vol. 11(11). P. 4427–4429 (****WoS Q1****, IF* 6.888*)*

2021

Kartsev A.I., Malkovsky S.I., Chibisov A.N. Analysis of Ionicity-Magnetism Competition in 2D-MX3 Halides towards a Low-Dimensional Materials Study Based on GPU-Enabled Computational Systems. // ***Nanomaterials 2021****. 11(11). 2967 (****WoS Q1****, IF 5.719)*

Gnidenko A.A., Chibisov A.N., Chibisova M.A., Prokhorenko A.V. Quantum mechanical modelling of phosphorus qubits in silicene under constrained magnetization. // ***RSC Advances. 2021****. 11. 33890-33894 (****WoS Q2, SCOPUS Q1****, IF 4.036)*

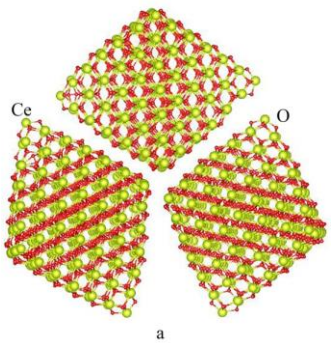
2022

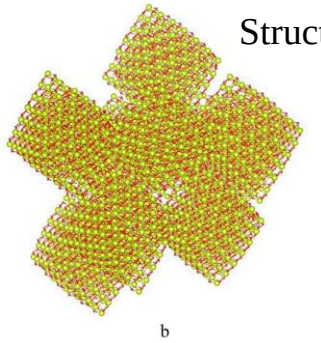
A.V. Goncharov, Chibisov A.N. Effect of External Pressure and Quantum State on the Local Magnetization of Germanium Layers: Ab Initio Calculation. // ***Advanced Theory and Simulations. 2023.*** *Vol. 12(13). P. 2244 (****WoS Q2****,* ***SCOPUS Q1****, IF 4.105)*

2023

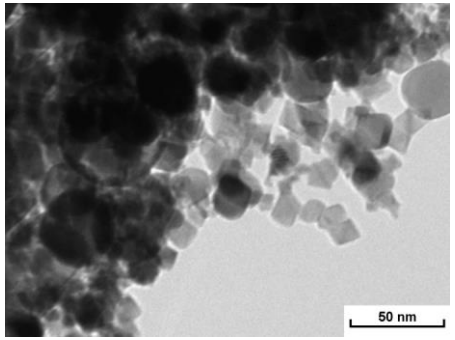
Chibisov A.N., *Gnidenko A.A.,* ***Chibisova M.A., Prokhorenko A.V.,*** *Yu Yang-Xin. Quantum-mechanical study of the optimal phosphorus atoms arrangement on silicene. //* ***Chemistry of Flat Materials****. 2023. Vol. 41. P. 100533 (****WoS Q2, SCOPUS Q1, IF 6.2****)*

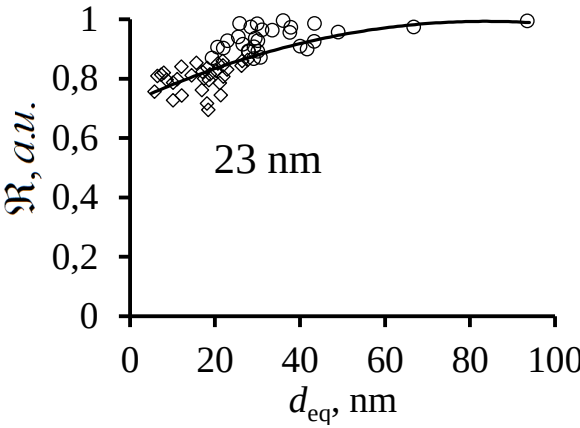
4. Effect of morphology and size on the thermodynamic stability of cerium oxide nanoparticles: Experiment and molecular dynamics calculation.

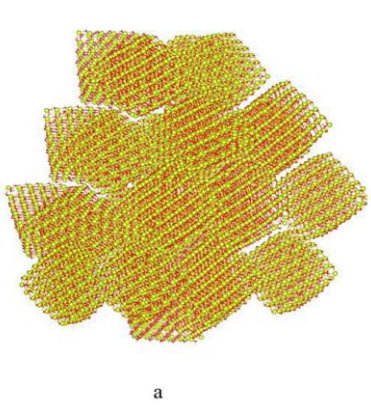


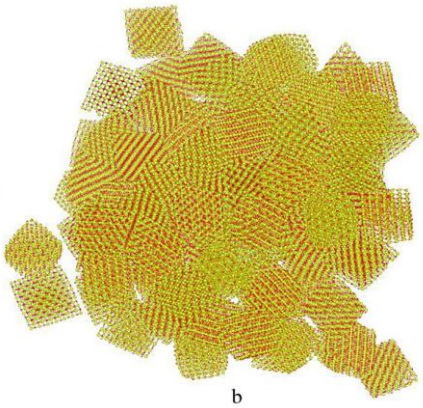


Structure of CeO2 nanoparticles: 4.7 nm (a) and 7.3 nm (b).







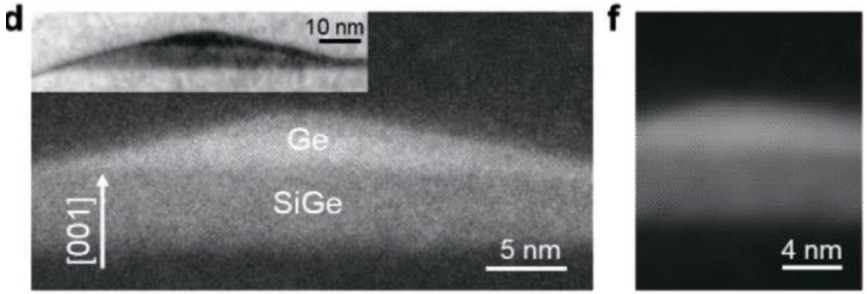


Structure of octahedral and spherical nanoparticles: (a) 10 nm in size and (b) 20.6 nm in size.

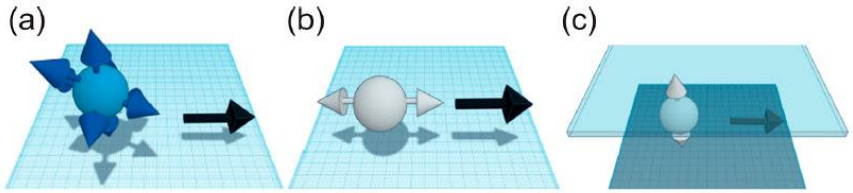
By means of the molecular dynamics method revealed the limiting dimensional transition from octahedral morphology to spherical shape in cerium oxide nanoparticles. The obtained results are relevant for technologists and experimenters in the field of controlled synthesis of nanostructured materials based on cerium oxide.

Chibisov A.N., Pugachevskii M.A., Kuzmenko A.P., Myo Min Than, **Kartsev A.I.** Effect of morphology and size on the thermodynamic stability of cerium oxide nanoparticles: Experiment and molecular dynamics calculation. // **Nanotechnology Reviews.** 2022. Vol. 11(1). P. 620-624. https://doi.org/10.1515/ntrev-2022-0038 (**WoS Q1, IF = 6.739**).

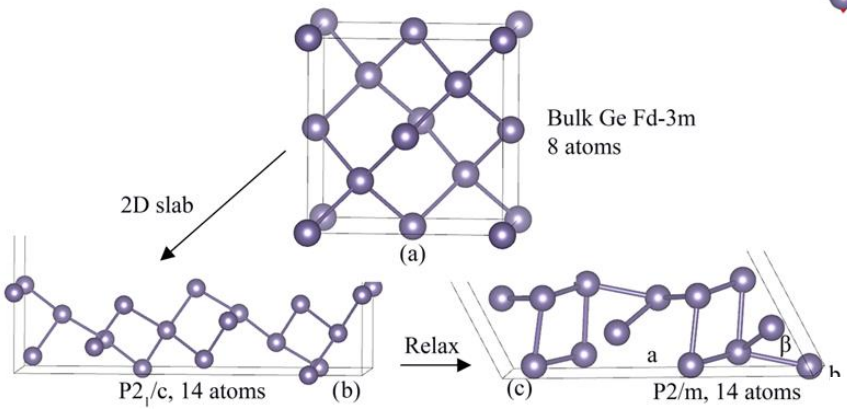
5 Analysis of spin states of hole qubits in a thin layer of germanium



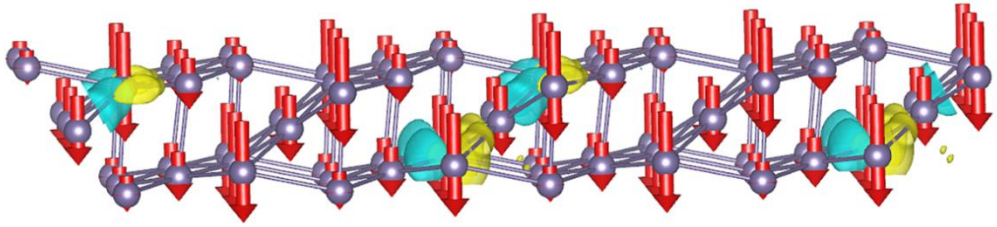
Fei Gao, et al. Adv. Mater. 2020, 1906523



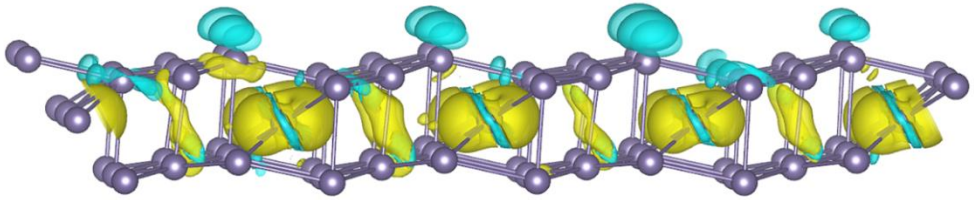
Georgios Katsaros, et al. Nano Lett. 2020, 20, 5201−5206



Chibisov A.N., Aleshin M.S., **Chibisova M.A.** DFT Analysis of Hole Qubits Spin State in Germanium thin layer. // **Nanomaterials**. 2022. Vol. 12(13). P. 2244 (**WoS Q1, IF 5.719**)



The localization of hole states (one hole) in germanium with quantum state |1>, with spin down direction s = –1, is the most energetically advantageous state by 0.72 μeV compared with the state |0>, with spin up s = +1.



Distribution of the difference in magnetization in the presence of a single hole. Yellow indicates states corresponding to |0> and blue indicates states corresponding to |1>.

Chibisov A.N., **Chibisova M.A., Prokhorenko A.V.**, et al. Possibilities of Controlling the Quantum States of Hole Qubits in an Ultrathin Germanium Layer Using a Magnetic Substrate: Results from ab Initio Calculations. // **Nanomaterials**. 2023. 13(23). P. 3070 (**WoS Q1, SCOPUS Q1, IF 5.3**)

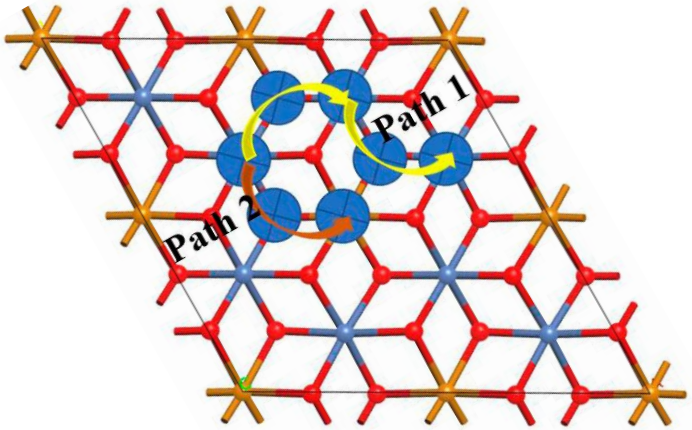
6 Theoretical calculation of the processes of ultrafast storage of sodium and potassium in Ni2TeO6: as a new promising cathode material.

The P2-type layered structures of A2Ni2TeO6 (where A = Na, K) are investigated as potential cathode materials for sodium and potassium storage using density functional theory calculations. The results of the work show that A2Ni2TeO6 is a promising cathode material for sodium and potassium storage, which may lead to the development of efficient and cost-competitive sodium-potassium-ion batteries.

Zhi-Hai Wu, Yang-Xin Yu, **A.N. Chibisov.** Density functional theory investigation on fast storage of sodium and potassium in Ni2TeO6 as a novel promising cathode material. // **Materials Today Energy.** 2023. Vol. 37. P. 101414. (**WoS Q1, IF 9.3**)

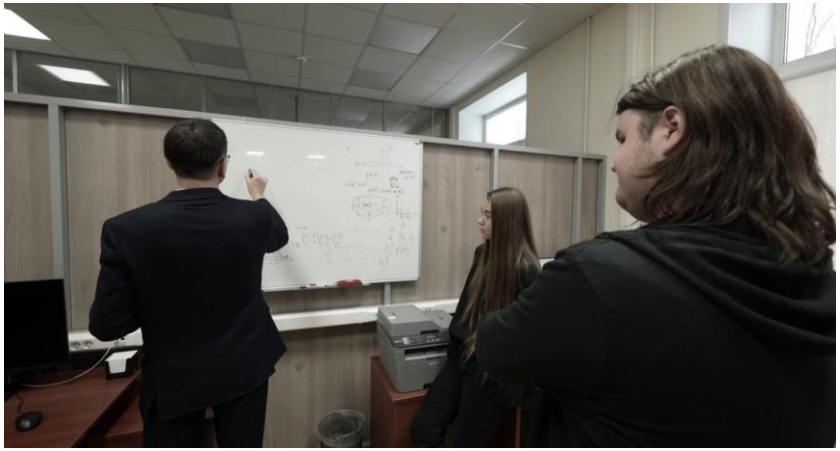
Tsinghua University

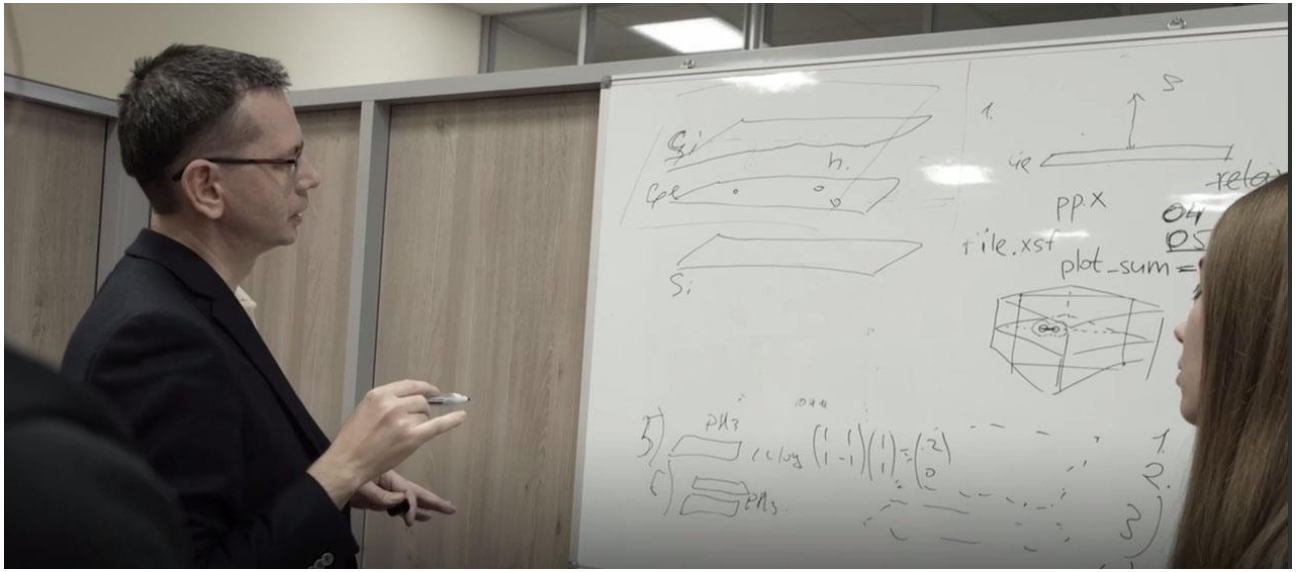
Computing Center of FEB RAS



Rongwei Shi, Yang-Xin Yu, **A.N. Chibisov.** Electrochemical reduction of cyanide on conjugated copper-organic framework Cu3(HHTP)2 monolayer: A dispersion-corrected DFT investigation. // **International Journal of Hydrogen Energy.** 2024. In Press (**WoS Q1, IF 7.2**)

Спасибо за внимание!





Andrey Chibisov. Ph.D.
Numerical method of mathematical physics Laboratory,
Computational Center, Russian Academy of Sciences, Khabarovsk, Russia
Web page: http://ru.linkedin.com/pub/andrey-chibisov/55/253/986/en