ЕВРОПЕЙСКИ СЪЮЗ
ЕВРОПЕЙСКИ ФОНД ЗА РЕГИОНАЛНО РАЗВИТИЕ

ЗАЕДНО СЪЗДАВАМЕ

ОПЕРАТИВНА ПРОГРАМА
НАУКА И ОБРАЗОВАНИЕ ЗА ИНТЕЛИГЕНТЕН РАСТЕЖ

Приложение на методите на изчислителната химия за моделиране на свойства и материали

Галя Маджарова

14.12.2022 г.

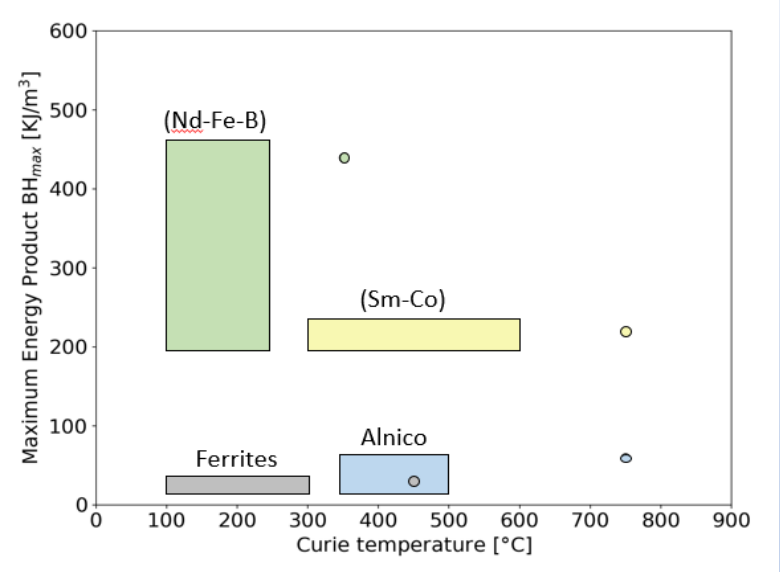
Център за високоефективни изчисления

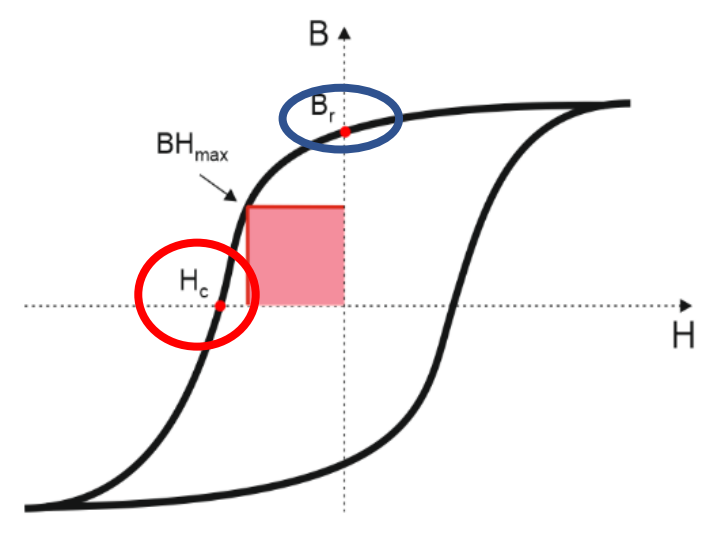
- 40 процесора (CPU) с общо 480 ядра
- графичните процесори (GPU) с общо 168 TFLOPS (SP) производителност
- INFINIBAND връзка.

Връзка
Структура – Състав – Свойства
за магнитни системи

Лаборатория по квантова и изчислителна химия, ФХФ, СУ

Твърди магнити без редкоземни елементи?





$$B = \mu_0(M + H)$$

$$(BH)_{max} = \frac{(B_r)^2}{4\mu_0}$$

$$(BH)_{max}^{EST} = \frac{(0.9\mu_0 M_s)^2}{4\mu_0}$$

$$M_r \leq 0.9 M_s$$

$$H_c > \frac{M_r}{2} > \frac{B_r}{2\mu_0}$$

B – магнитната индукция
M – намагнитването
H – външното магнитно поле,
μ_0 – магнитната проницаемост на вакуума
MAE – енергия на магнитна анизотропия

$$H_c \sim \frac{MAE}{\mu_0 M_r}$$

M_s MAE

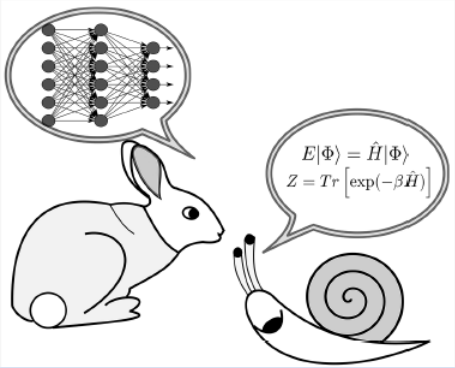
- елементно съдържание
- кристална структура
- магнитна подредба

B_r H_c T_c BH_{max}

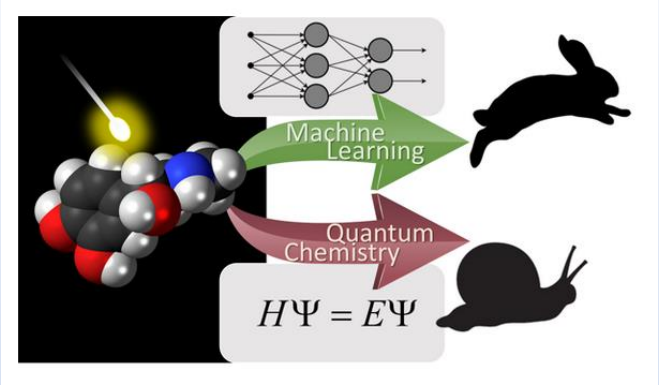
- дефекти
- размер на кристалитите
- форма и ориентация на кристалните зърна
- напрежения на границите
- техника на производство

Quantum Chemistry

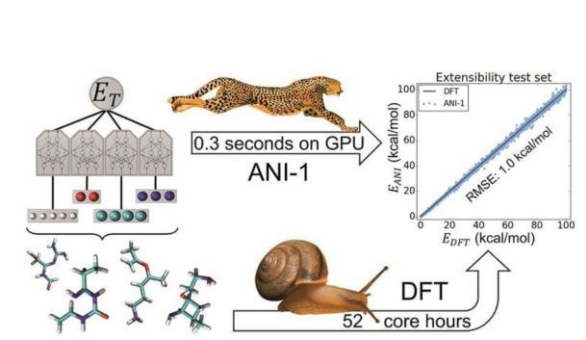
Machine Learning



Chem. Rev. 2021, 121, 9816−9872



https://anscse25.com/plenary-speakers/



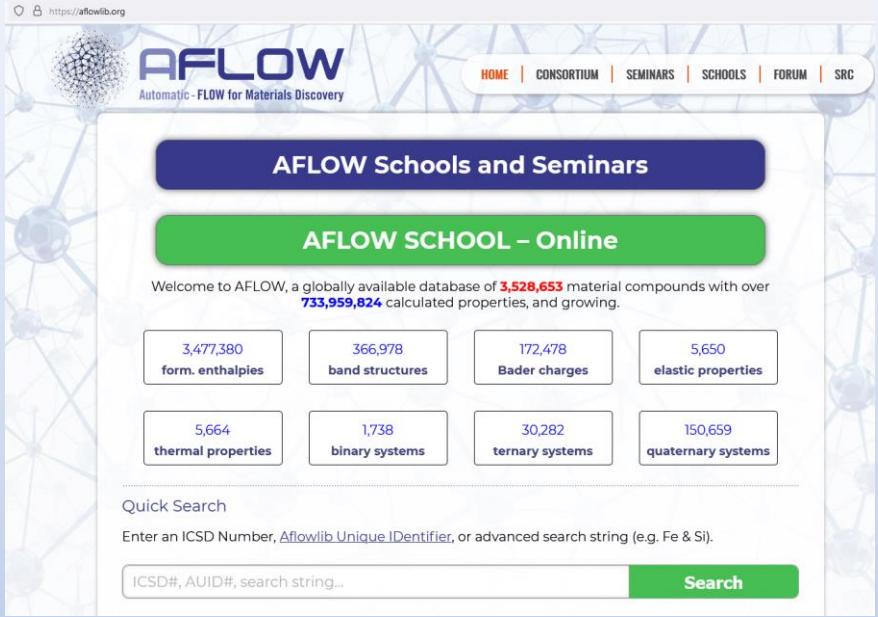
https://roitberg.chem.ufl.edu/research/

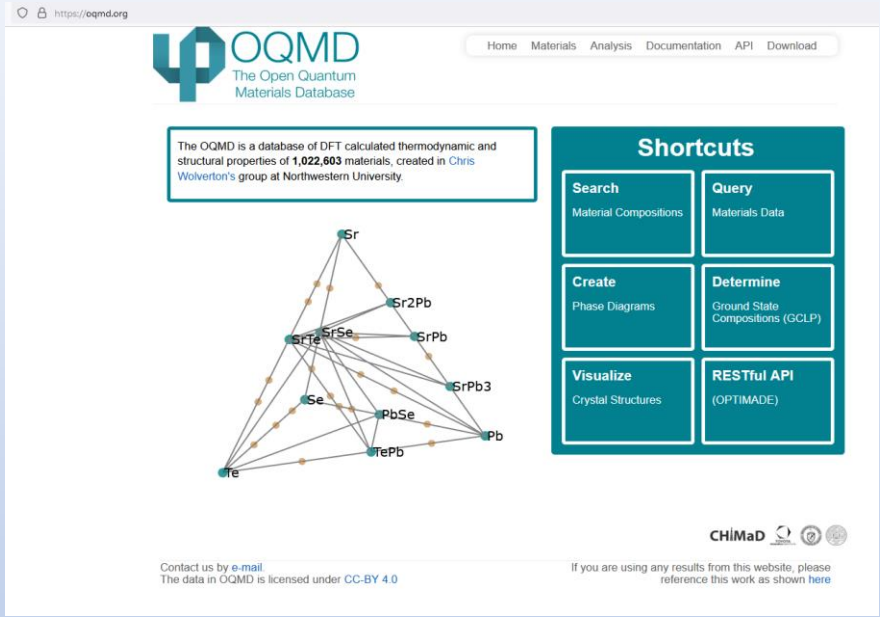
Машинно обучение

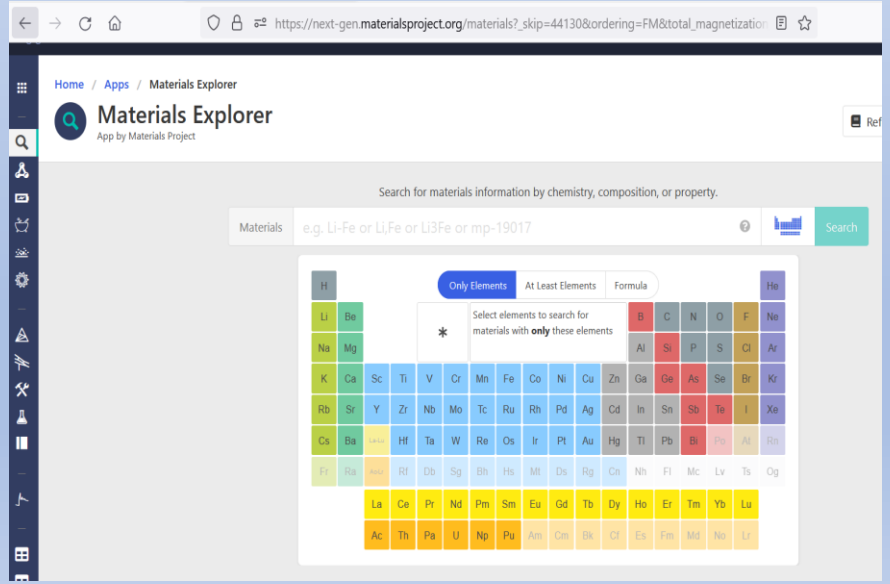
Квантовохимични изчисления

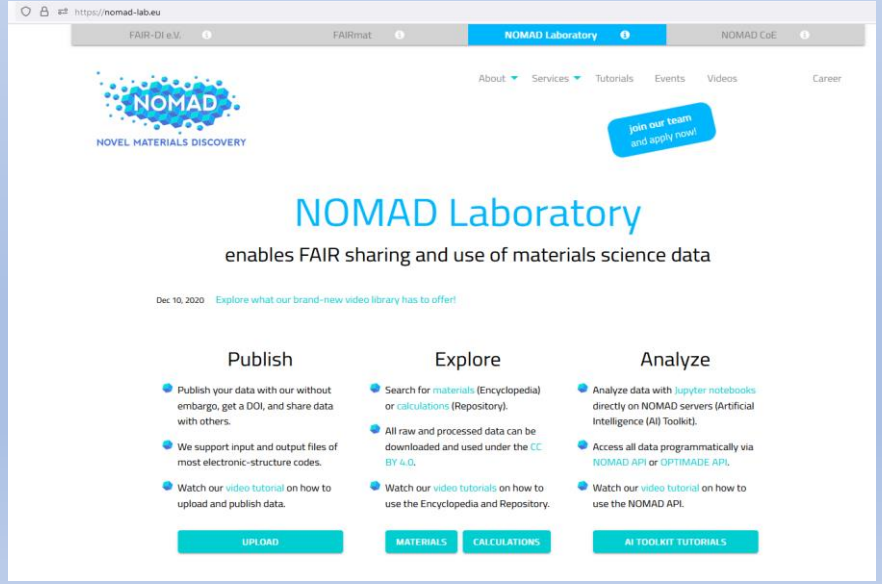
Експеримент

Бази данни


https://aflowlib.org
AFLOW
Automatic - FLOW for Materials Discovery
HOME | CONSORTIUM | SEMINARS | SCHOOLS | FORUM | SRC
AFLOW Schools and Seminars
AFLOW SCHOOL – Online
Welcome to AFLOW, a globally available database of 3,528,653 material compounds with over 733,959,824 calculated properties, and growing.
3,477,380 form. enthalpies
366,978 band structures
172,478 Bader charges
5,650 elastic properties
5,664 thermal properties
1,738 binary systems
30,282 ternary systems
150,659 quaternary systems
Quick Search
Enter an ICSD Number, Aflowlib Unique IDentifier, or advanced search string (e.g. Fe & Si).
ICSD#, AUID#, search string...
Search

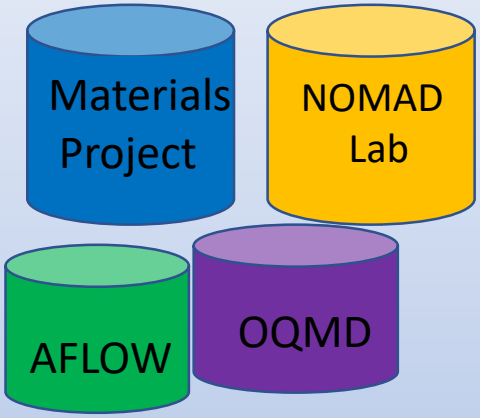

https://oqmd.org
OQMD
The Open Quantum Materials Database
Home Materials Analysis Documentation API Download
The OQMD is a database of DFT calculated thermodynamic and structural properties of 1,022,603 materials, created in Chris Wolverton's group at Northwestern University.
Shortcuts
Search
Material Compositions
Query
Materials Data
Create
Phase Diagrams
Determine
Ground State Compositions (GCLP)
Visualize
Crystal Structures
RESTful API
(OPTIMADE)
Sr
Sr2Pb
SrTe
SrSe
SrPb
SrPb3
Se
PbSe
Pb
TePb
Te
CHiMaD
Contact us by e-mail.
The data in OQMD is licensed under CC-BY 4.0
If you are using any results from this website, please reference this work as shown here


https://next-gen.materialsproject.org/materials?_skip=44130&ordering=FM&total_magnetizatio
Home / Apps / Materials Explorer
Materials Explorer
App by Materials Project
Search for materials information by chemistry, composition, or property.
Materials
e.g. Li-Fe or Li,Fe or Li3Fe or mp-19017
Search
Only Elements
At Least Elements
Formula
Select elements to search for materials with only these elements

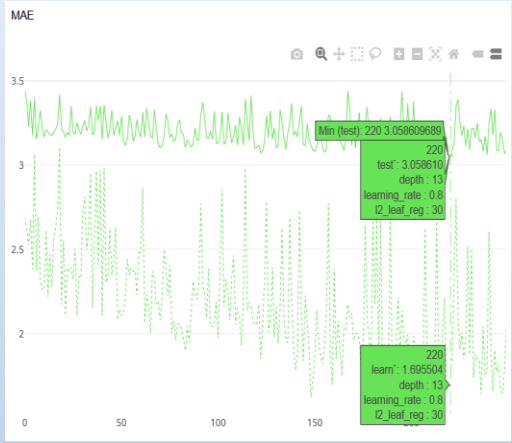

https://nomad-lab.eu
FAIR-DI e.V.
FAIRmat
NOMAD Laboratory
NOMAD CoE
NOMAD
NOVEL MATERIALS DISCOVERY
About Services Tutorials Events Videos Career
join our team and apply now!
NOMAD Laboratory
enables FAIR sharing and use of materials science data
Dec 10, 2020 Explore what our brand-new video library has to offer!
Publish
Publish your data with our without embargo, get a DOI, and share data with others.
We support input and output files of most electronic-structure codes.
Watch our video tutorial on how to upload and publish data.
Explore
Search for materials (Encyclopedia) or calculations (Repository).
All raw and processed data can be downloaded and used under the CC BY 4.0.
Watch our video tutorials on how to use the Encyclopedia and Repository.
Analyze
Analyze data with Jupyter notebooks directly on NOMAD servers (Artificial Intelligence (AI) Toolkit).
Access all data programmatically via NOMAD API or OPTIMADE API.
Watch our video tutorial on how to use the NOMAD API.
UPLOAD
MATERIALS
CALCULATIONS
AI TOOLKIT TUTORIALS

Етапи на машинното обучение

Извличане на данни → **Избор на параметри** → **Машинно обучение**



	A	n	I	X	R	M	D	A_mm	n_mm	I_mm	X_mm	R_mm	M_mm	D_mm
A														
n	0.17													
I	-0.01	0.01												
X	0.20	-0.05	0.87											
R	0.11	0.17	-0.70	-0.75										
M	0.28	0.29	-0.39	-0.39	0.80									
D	0.18	0.32	-0.02	0.02	0.01	0.10								
A_mm	0.50	0.04	0.26	0.32	-0.11	0.10	-0.00							
n_mm	-0.00	0.28	-0.17	-0.15	0.12	0.07	0.03	0.06						
I_mm	-0.13	-0.08	0.74	0.59	-0.45	-0.29	0.03	0.19	0.01					
X_mm	0.07	-0.09	0.50	0.47	-0.26	-0.11	0.09	0.32	0.08	0.80				
R_mm	-0.01	-0.04	0.21	0.17	-0.21	-0.27	0.26	0.04	0.18	0.53	0.66			
M_mm	0.09	-0.03	0.02	0.05	-0.10	0.05	0.08	0.20	0.26	0.17	0.30	0.47		
D_mm	0.20	-0.10	0.21	0.29	-0.14	0.16	-0.09	0.38	0.08	0.20	0.29	0.03	0.51	
magnetization	-0.10	0.17	0.04	0.01	-0.09	-0.13	0.24	-0.02	-0.06	0.03	0.02	0.17	0.01	-0.13



Бази данни

- High-throughput screening
- Експериментални данни
- Индивидуални данни от изчисления

126 335 съединения → **7 961 съединения**

Независими параметри

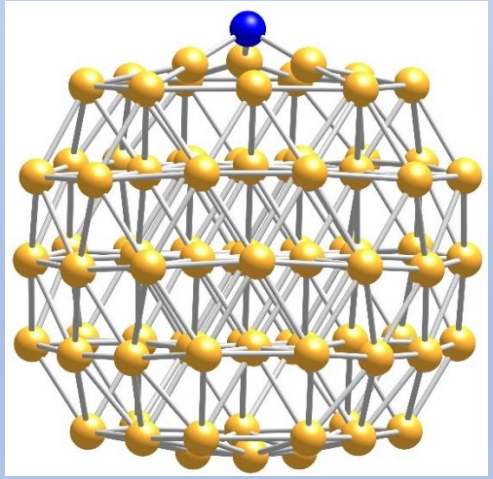
- Automated feature engineering
- Избор въз основа на предварителна информация

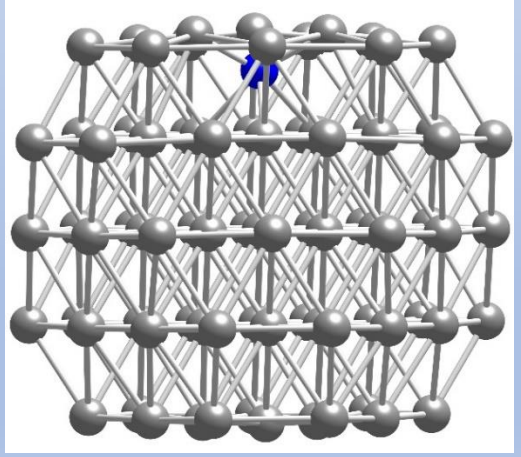
Модел

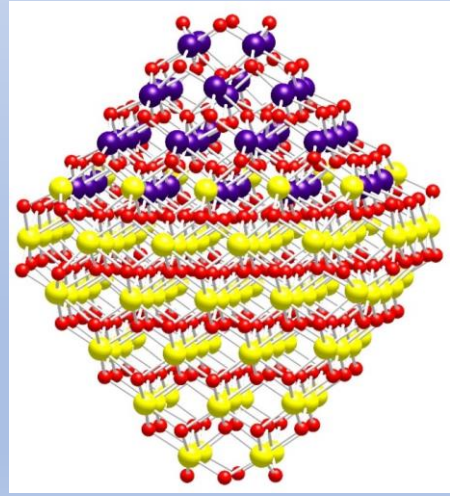
(6%) остават за обучение и валидиране

Квантовохимично моделиране на структурата и свойствата на оксидни наночастици

- Биметални наночастици въз основата на CeO_2: повишаване на потенциала им в реакции на каталитично окисление
- Влияние на примесни атоми от каталитични реакции върху каталитичната активност златни и сребърни наноклъстери

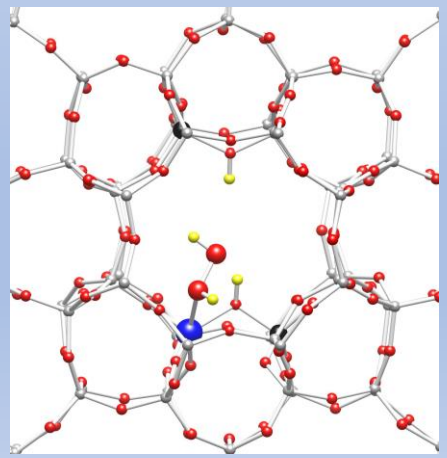






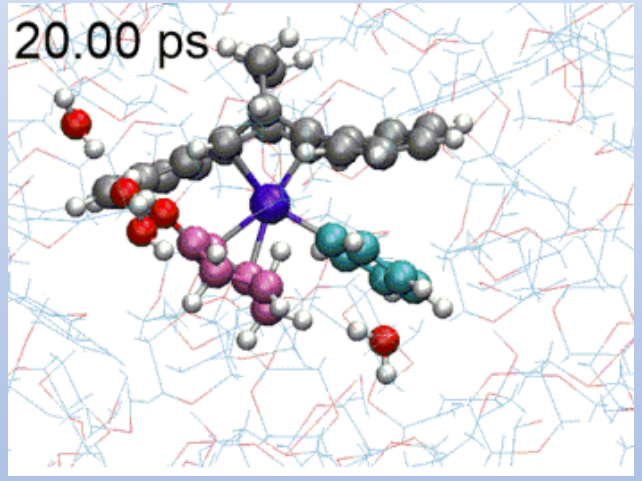
Квантовохимично моделиране на структурата и реакционната способност на каталитични центрове в зеолити

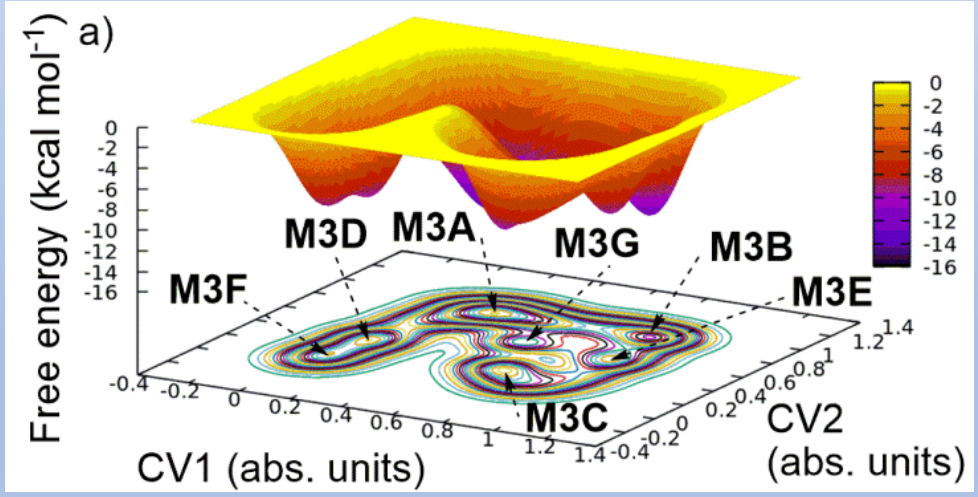
- Формиране и миграция на дефекти в зеолитните решетки.
- Изоморфно заместване на Si^{4+} с Ti^{4+}, Ge^{4+}, Zr^{4+}, Al^{3+} йони в зеолитната решетка.
- Формиране на катлитични активни комплекси в кухините на заеолитната решетка.
- Симулиране на спектроскопски характеристики на каталитично активни центрове в зеолитните канали.



Приложение на ab-initio молекулна динамика и метадинамика за изследване на профил на свободната енергия

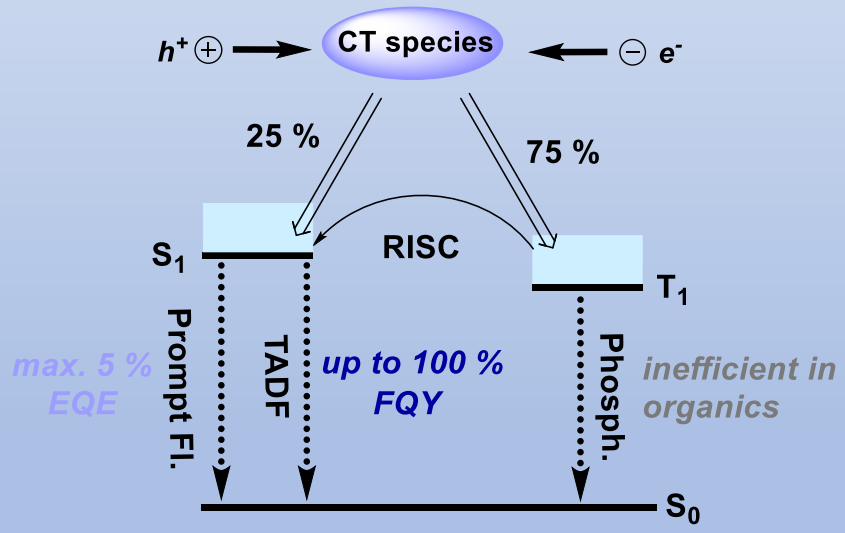
- Енантиоселективни хомогенно каталитични реакции базирани на Rh комплекси
- Създаване на реалистични модели за изследване на каталитичния цикъл

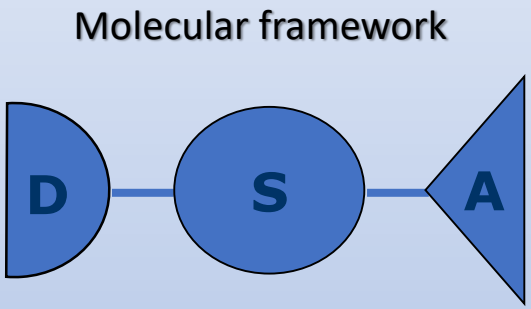


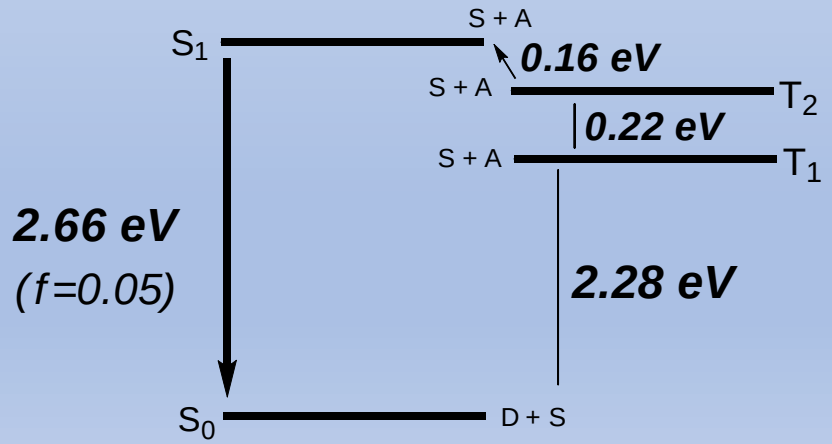


Квантовохимично моделиране на сини TADF емитери за OLED

- Намиране на нови структури
- Увеличаване на ефективността на вече съществуващи структури чрез изследване на нови акцептори и донори







Благодаря за вниманието!

Всички изчисления свързани с изследванията са направени на високопроизводителен клъстер в рамките на проект ЦВП "Национален център по мехатроника и чисти технологии", BG05M2OP001-1.001-0008", Европейския фонд за регионално развитие в рам-ките на Оперативна програма "Наука и образование за интели-гентен растеж 2014 - 2020".