



Konferencija Srce DEI

Otkrivanje novih materijala u AI doba

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Institut Ruđer Bošković

Srce DEI 2026

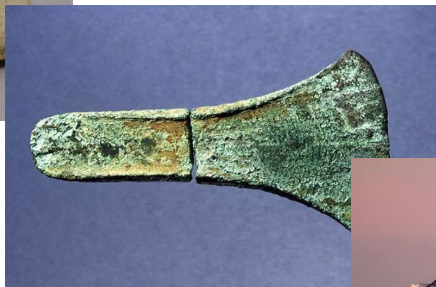




Materijali definiraju čovječanstvo



Kameno doba



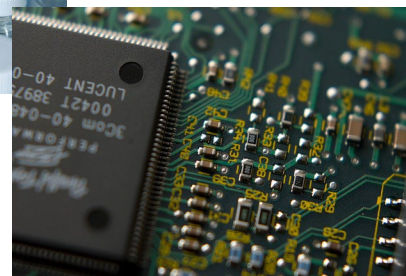
Brončano doba



Željezno doba /
Doba čelika



Doba plastike



Doba silicija

???



... i definirat će našu budućnost ...



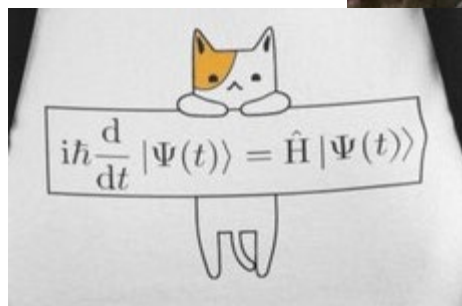


... i definirat će našu budućnost ...



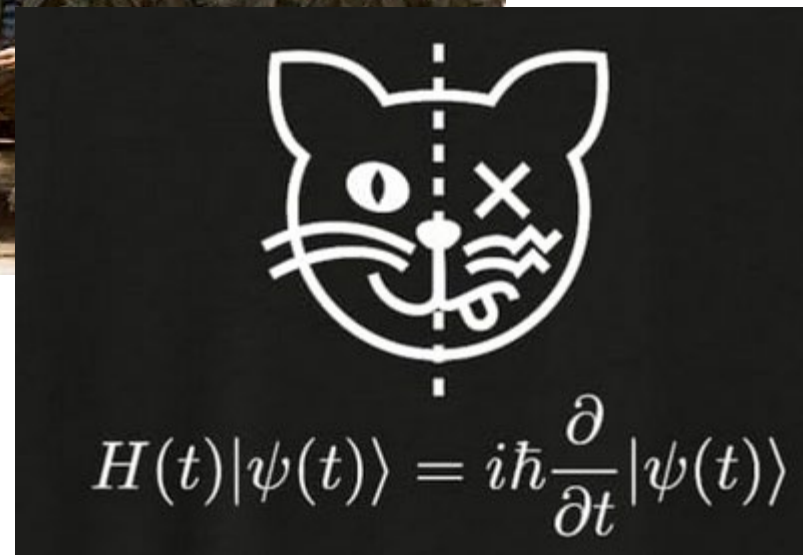


Fizikalni zakoni su poznati 100 godina



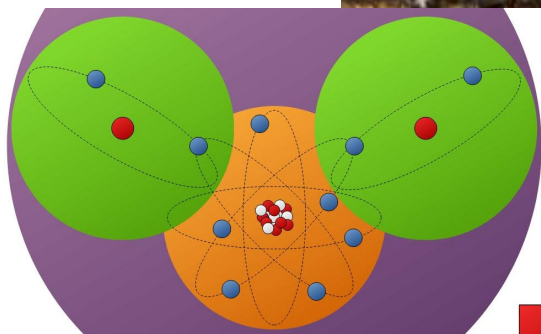
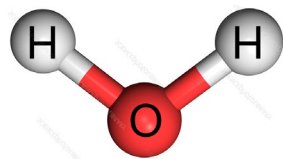
$$\hat{H}\Psi = E\Psi$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$$





Fizikalni zakoni su poznati 100 god., ali...



1 čestica u 3D: $100^3=10^6$
10 čestica: $100^{3 \times 10}=10^{30}$
100 čestica: $100^{300}=10^{600}$

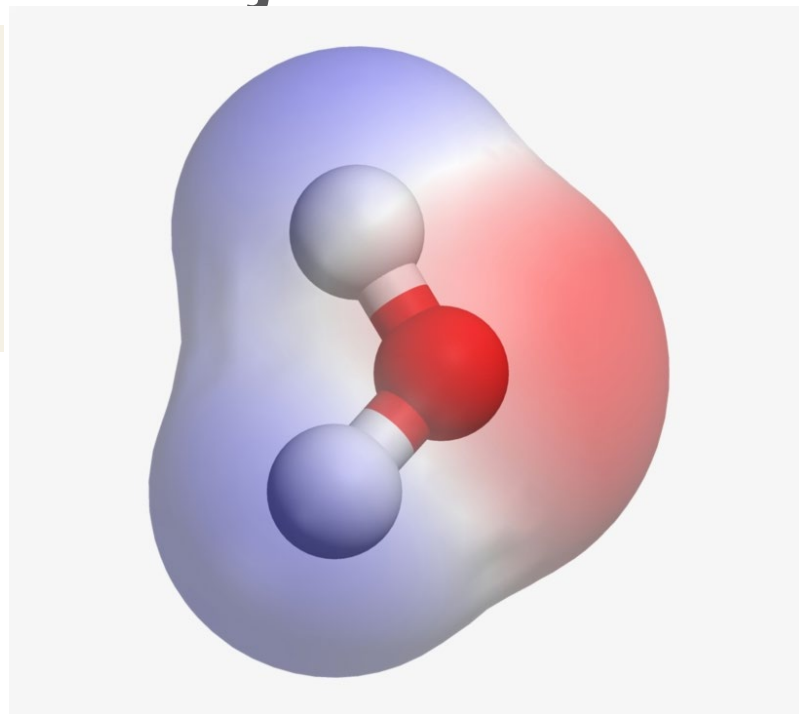
$$F = k \frac{q_1 q_2}{r^2}$$

$$\Psi(r_1, \dots, r_{N_e}; R_1, \dots, R_{N_n})$$

$$i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \frac{-\hbar^2}{2m} \nabla^2 \Psi(r, t) + V(r) \Psi(r, t)$$



Srećom imamo jako dobre aproksimacije



TOP TEN CITED PAPERS

Just 3 papers have more than 200,000 citations each, according to the Web of Science database. All three cover biological laboratory techniques. This update to a 2014 list of most-cited articles shows that the top three papers remain unchanged. But there have been shifts in the positions of others (triangles), and some additions that were not on the previous list (orange stars). For alternative rankings from two other databases, and a median ranking across all three, see Supplementary information (go.nature.com/425g9dn).

1	355,968 citations
	<i>Protein measurement with the folin phenol reagent</i> (1951)
2	259,187
	<i>Cleavage of structural proteins during the assembly of the head of bacteriophage T4</i> (1970)
3	242,864
	<i>A rapid and sensitive method for the quantitation of microgram quantities of protein utilizing the principle of protein-dye binding</i> (1976)
▲ 4 (16)	174,137
	<i>Generalized gradient approximation made simple</i> (1996)
▲ 5 (21)	148,626
	<i>Analysis of relative gene expression data using real-time quantitative PCR and the 2^{-ΔΔC_t} method</i> (2001)
★ 6	133,965
	<i>Preferred reporting items for systematic reviews and meta-analyses: the PRISMA statement</i> (2009)*
★ 7	116,706
	<i>Deep residual learning for image recognition</i> (2016, preprint 2015)
▲ 8 (43)	101,906
	<i>Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set</i> (1996)
★ 9	100,327
	<i>Using thematic analysis in psychology</i> (2006)*
▼ 10 (7)	93,223
	<i>Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density</i> (1988)

Data show citations from Web of Science "Core Collection" journals as of March 2025, to permit comparison with 2014 list (*Nature* 514, 550–553; 2014). Orders would change if citation metrics from other databases were included (see Supplementary information).

*Paper was published in multiple journals simultaneously. This total aggregates citations to all journal versions.

*Corrected for data error in Web of Science, which lists a different paper by the same authors.

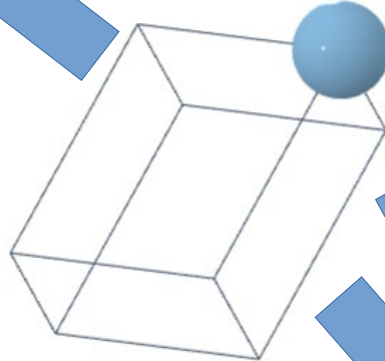
©nature

Teorija funkcionala gustoće: valna funkcija ovisi o $3N$ koordinata - gustoća elektrona o samo 3 prostorne koordinate

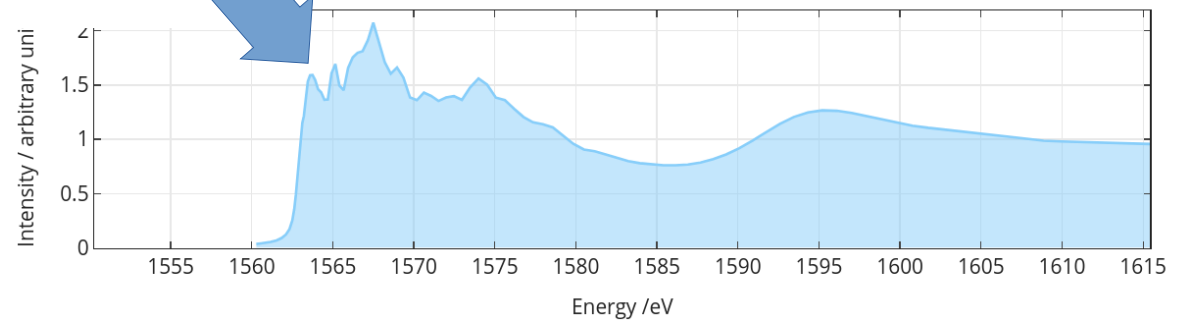
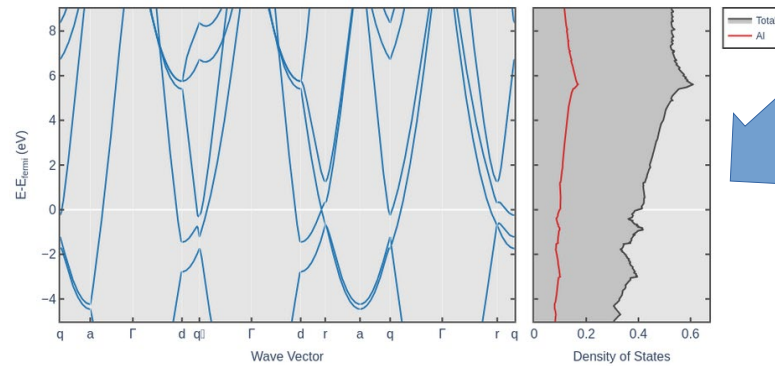
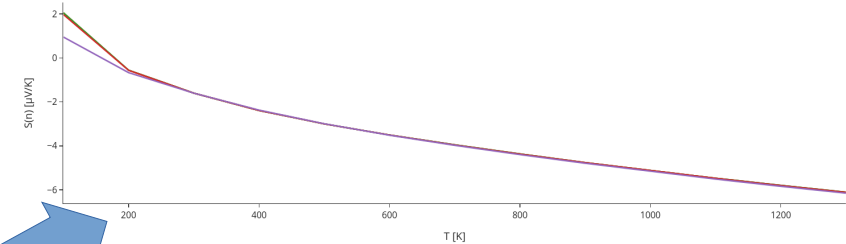


Dizajn ab initio - iz prvih principa

Stiffness Tensor (GPa)

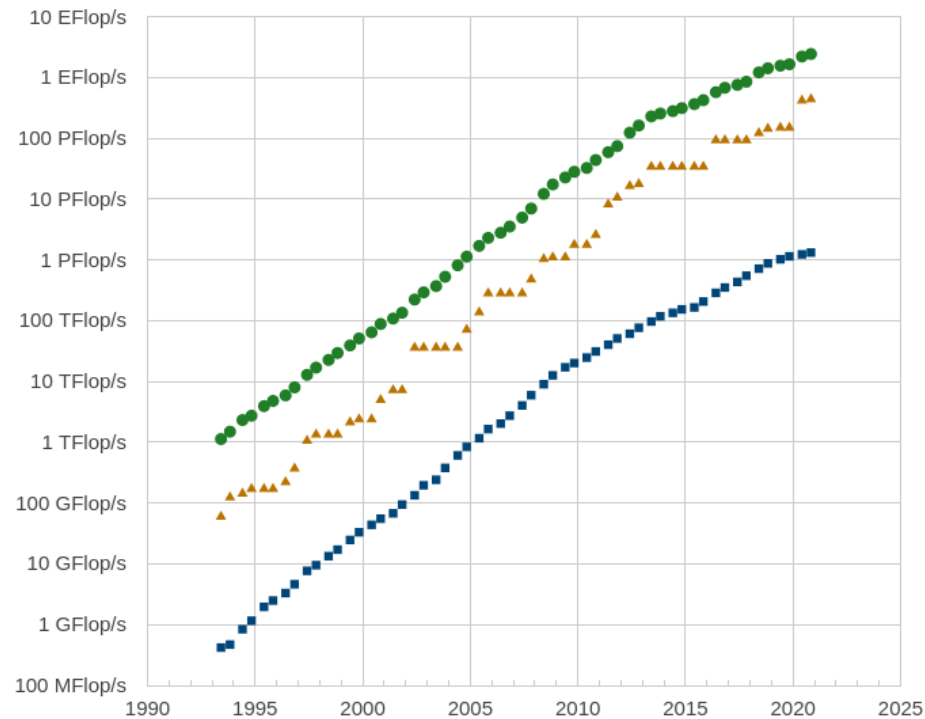
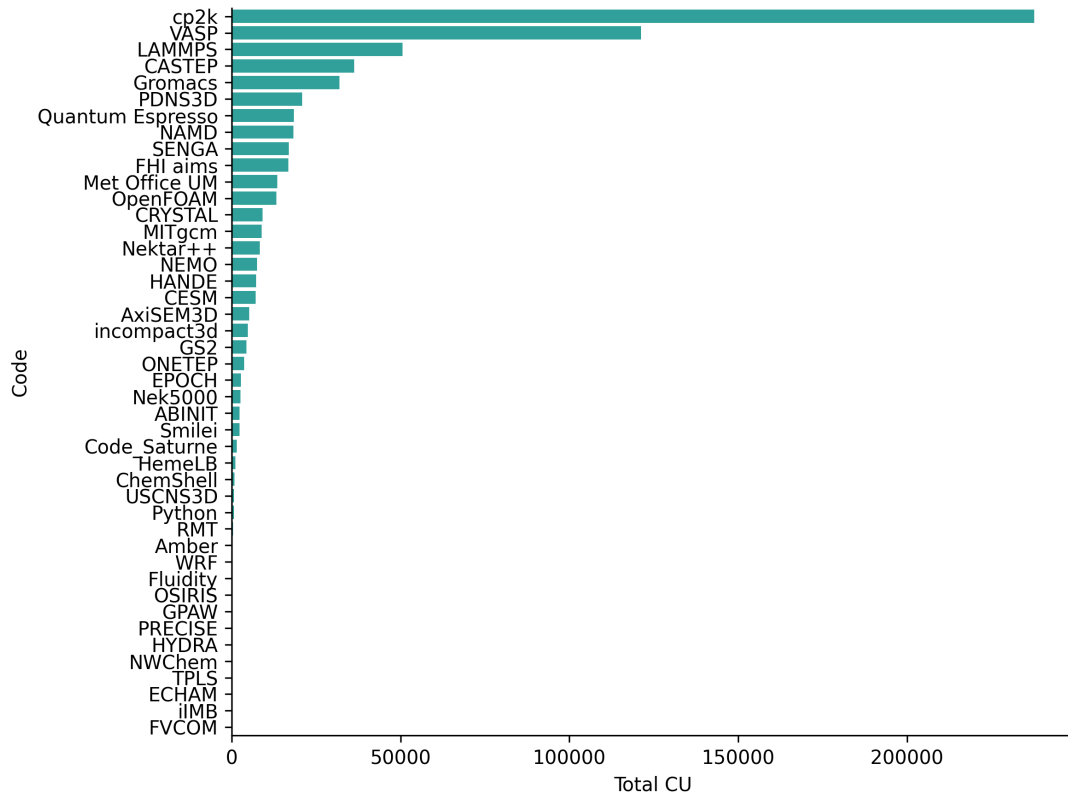
$$\begin{bmatrix} 47 & 12 & 12 & 0 & 0 & 0 \\ 12 & 47 & 12 & 0 & 0 & 0 \\ 12 & 12 & 47 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 12 \end{bmatrix}$$


Temperature- and Doping-Level-Dependence of n-type Seebeck Coefficient





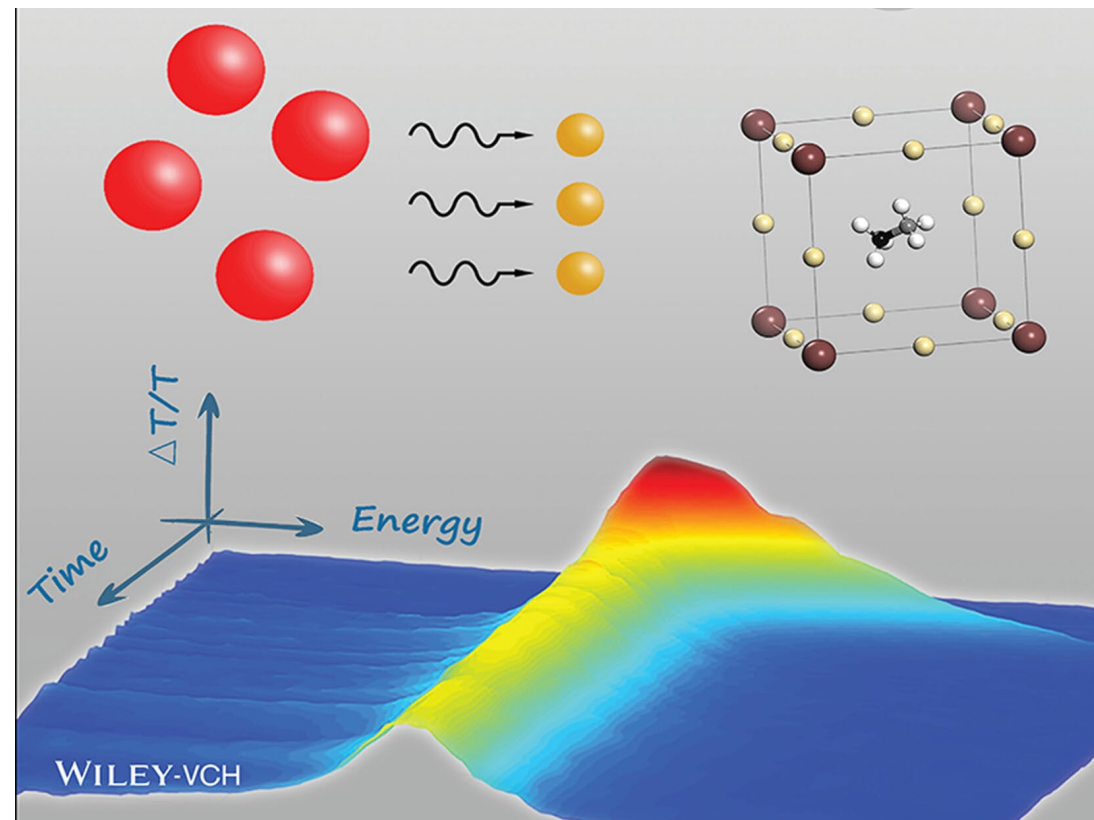
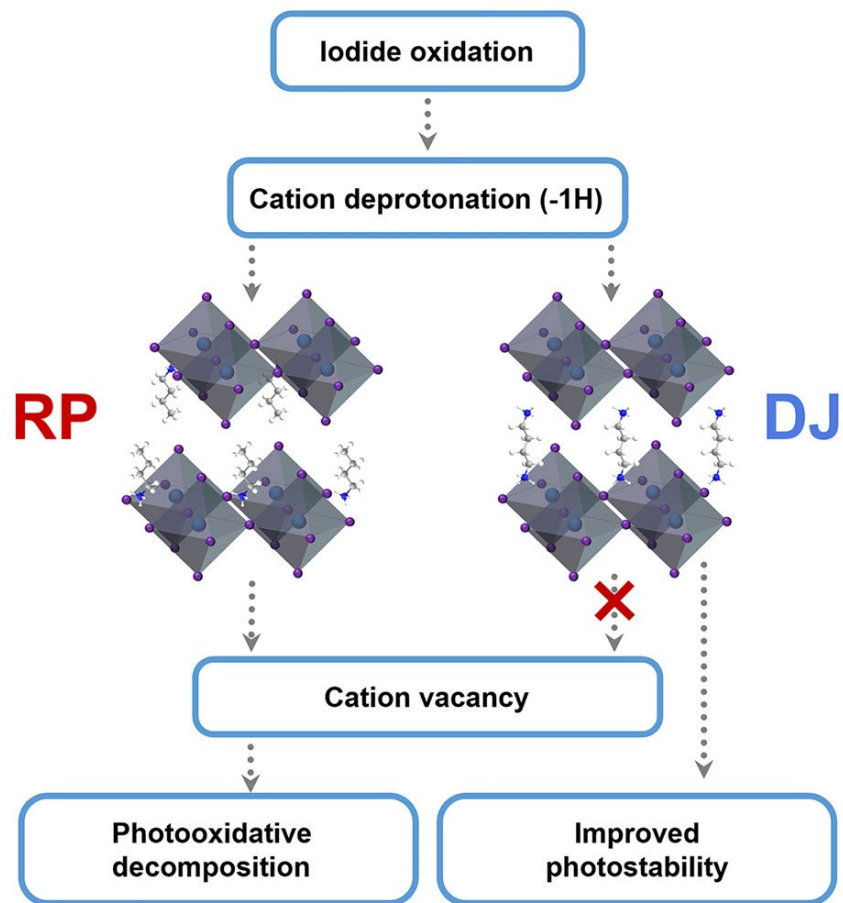
DFT i dalje skup, superračunala sve jača



Na Supeku / Padobranu također >50% resursa odlazi na DFT

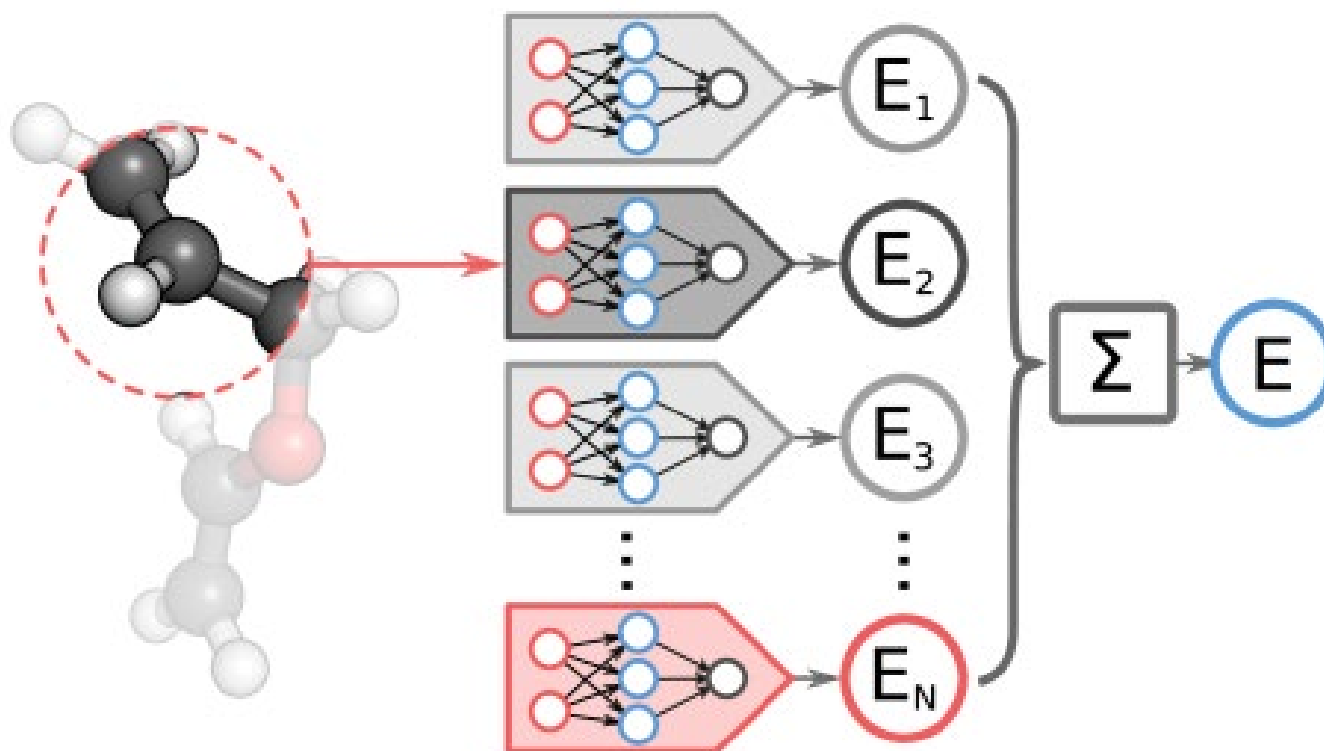


DFT nam pruža atomistički uvid





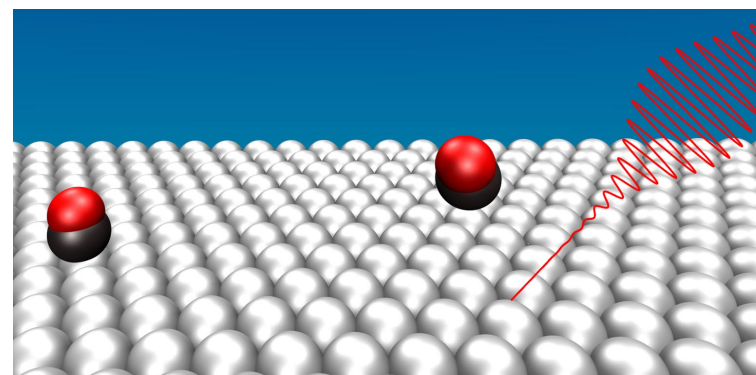
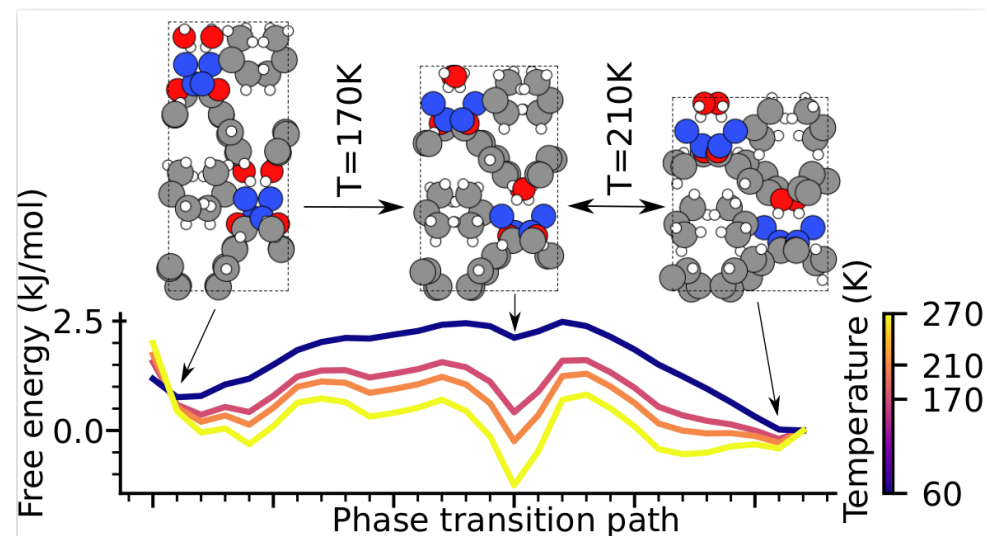
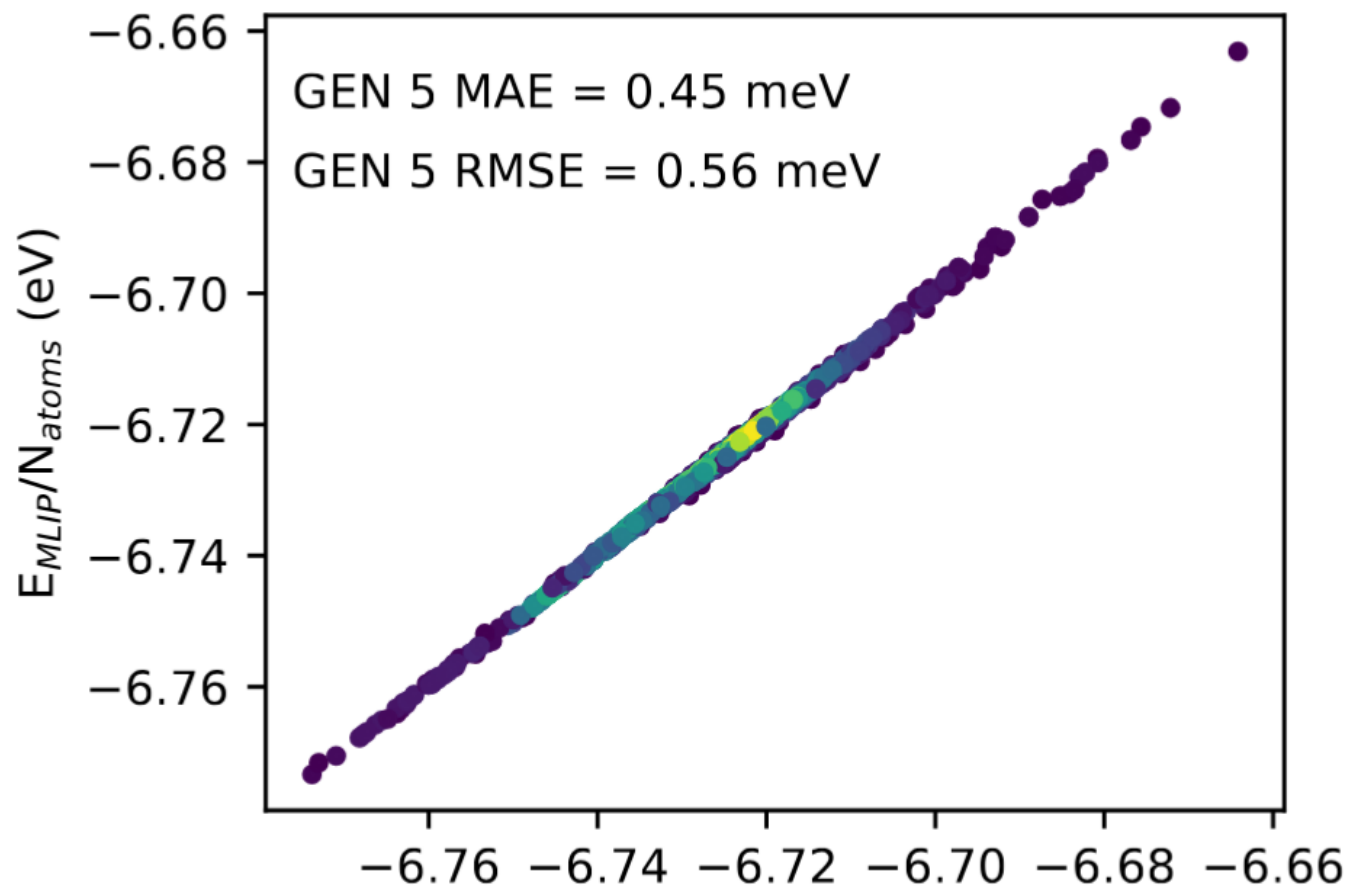
Potreba za bržim metodama



Ideja: Naučiti DFT rješenja za bilo koji materijal pomoću strojnog učenja, dobiti točan model koji je nekoliko redova veličine brži

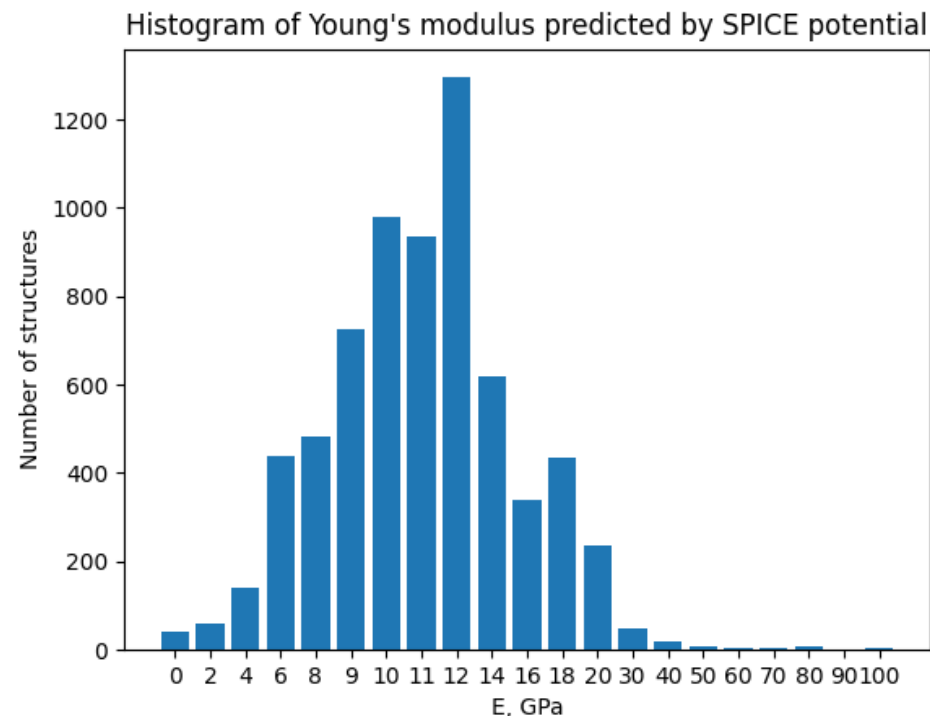
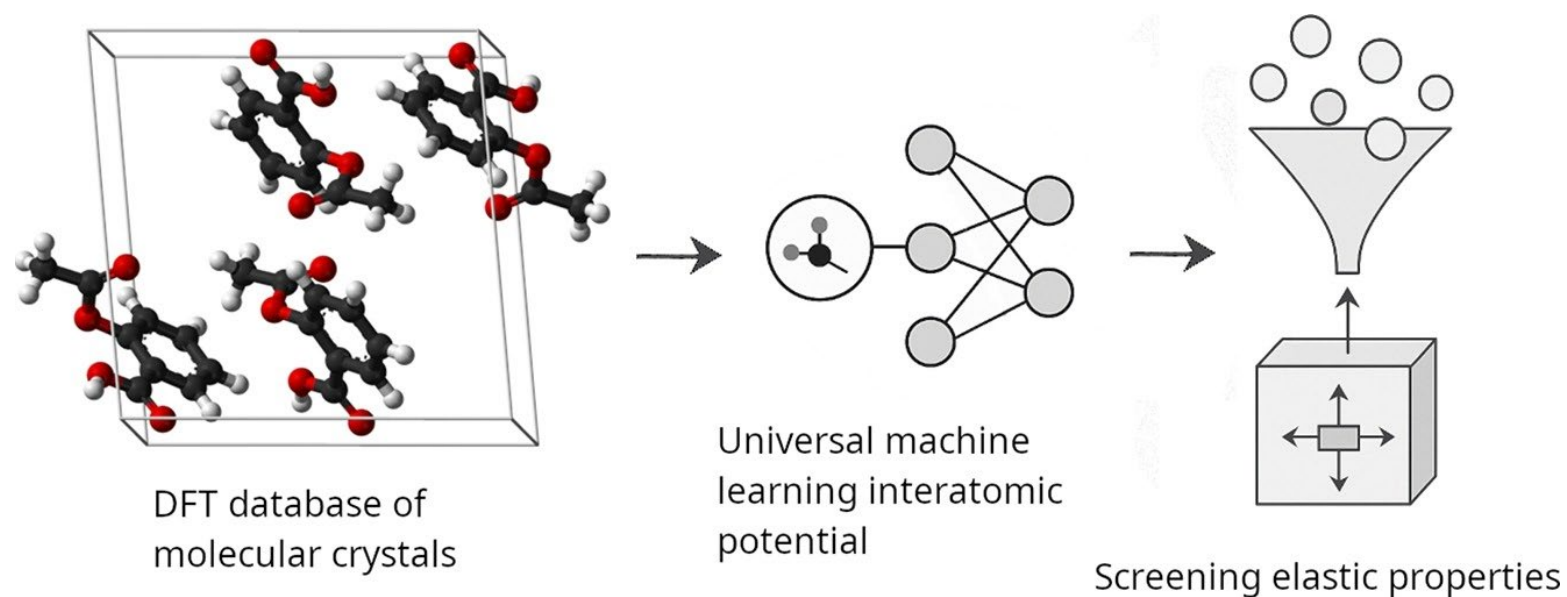


Radi odlično za predikciju E/F/dinamike





Model za molekularne materijale

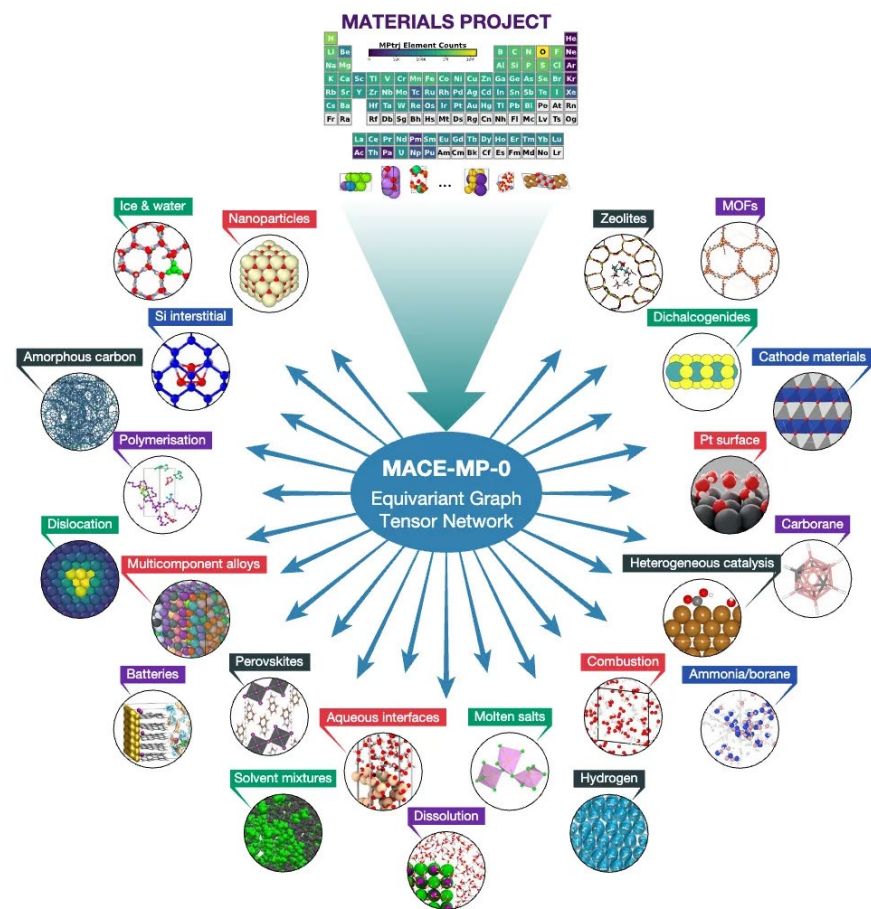


Ekvivarijantna graf neuralna mreža s 4.7M parametara trenirana na 2M DFT računa za molekule na Supeku ~ 2 tjedna na 4xA100



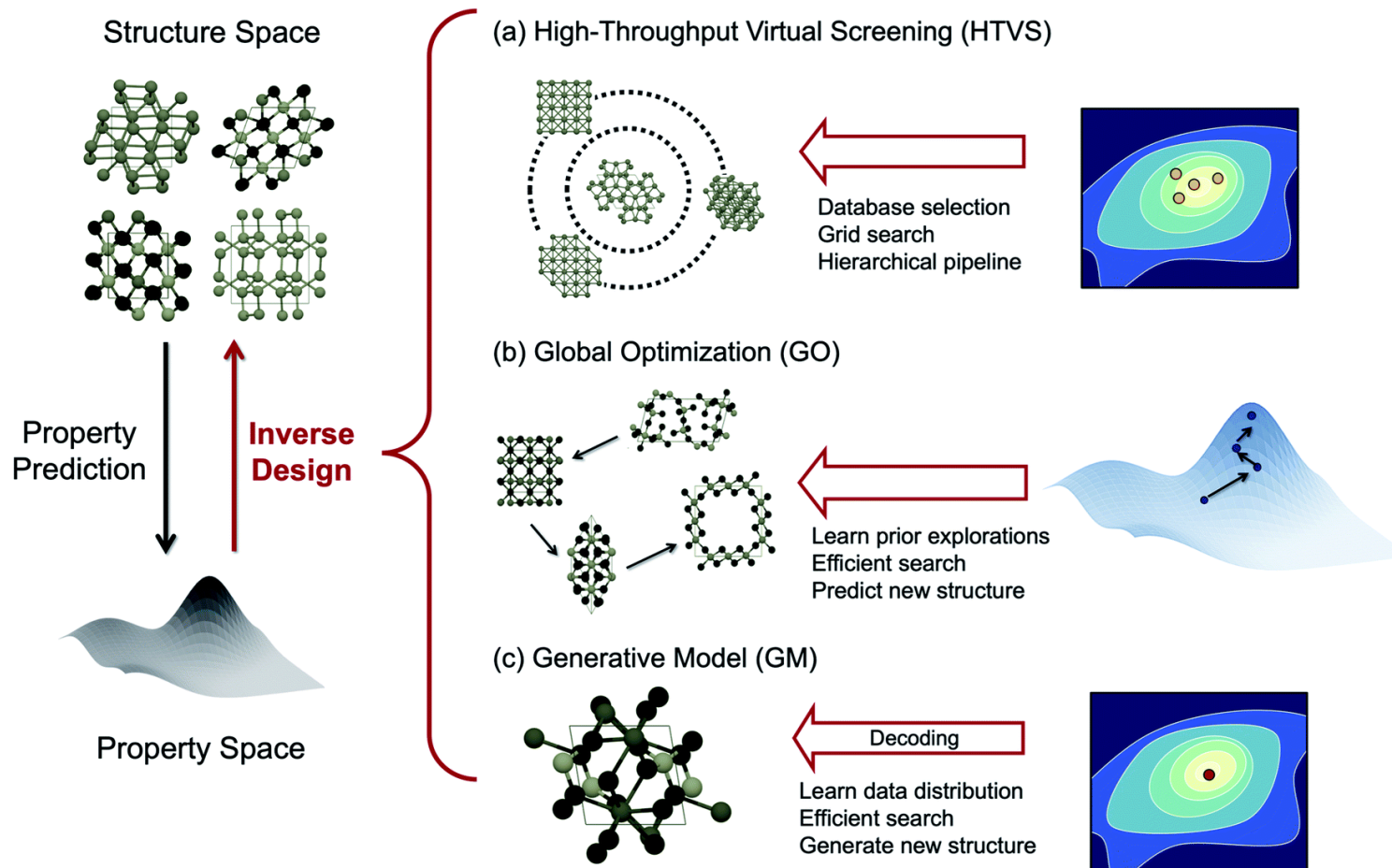
Trenutno utrka za univerzalnim modelom

Model	Org	Date Added	Params	Training Set	F1 ↑
eSEN-30M-OAM		2025-03-17	30.2M	6.6M (113M) OMat24+MPtrj+sAlex	0.925
EquFlash		2025-06-23	28.7M	6.6M (113M) OMat24+MPtrj+sAlex	0.919
eqV2 M		2024-10-18	86.6M	3.37M (102M) OMat24+MPtrj	0.917
Nequip-OAM-XL		2025-11-30	32.1M	6.6M (113M) OMat24+sAlex+MPtrj	0.906
ORB v3		2025-04-05	25.5M	6.47M (133M) MPtrj+Alex+OMat24	0.905
SevenNet-MF-ompa		2025-03-13	25.7M	6.6M (113M) OMat24+sAlex+MPtrj	0.901
AlphaNet-v1-OMA		2025-05-12	4.65M	6.6M (113M) OMat24+sAlex+MPtrj	0.901
Allegro-OAM-L		2025-09-08	9.7M	6.6M (113M) OMat24+sAlex+MPtrj	0.895
Nequip-OAM-L		2025-09-08	9.6M	6.6M (113M) OMat24+sAlex+MPtrj	0.893
DPA-3.1-3M-FT		2025-06-05	3.27M	163M OpenLAM	0.884
GRACE-2L-OAM-L		2025-09-09	26.4M	6.6M (113M) OMat24+sAlex+MPtrj	0.883
GRACE-2L-OAM		2025-02-06	12.6M	6.6M (113M) OMat24+sAlex+MPtrj	0.880
ORB v2		2024-10-11	25.2M	3.25M (32.1M) MPtrj+Alex	0.880
MatterSim v1 5M		2024-12-16	4.55M	17M MatterSim	0.862
MACE-MPA-0		2024-12-09	9.06M	3.37M (12M) MPtrj+sAlex	0.852
eSEN-30M-MP		2025-03-17	30.1M	146k (1.58M) MPtrj	0.831
GNoME		2024-02-03	16.2M	6M (89M) GNoME	0.829



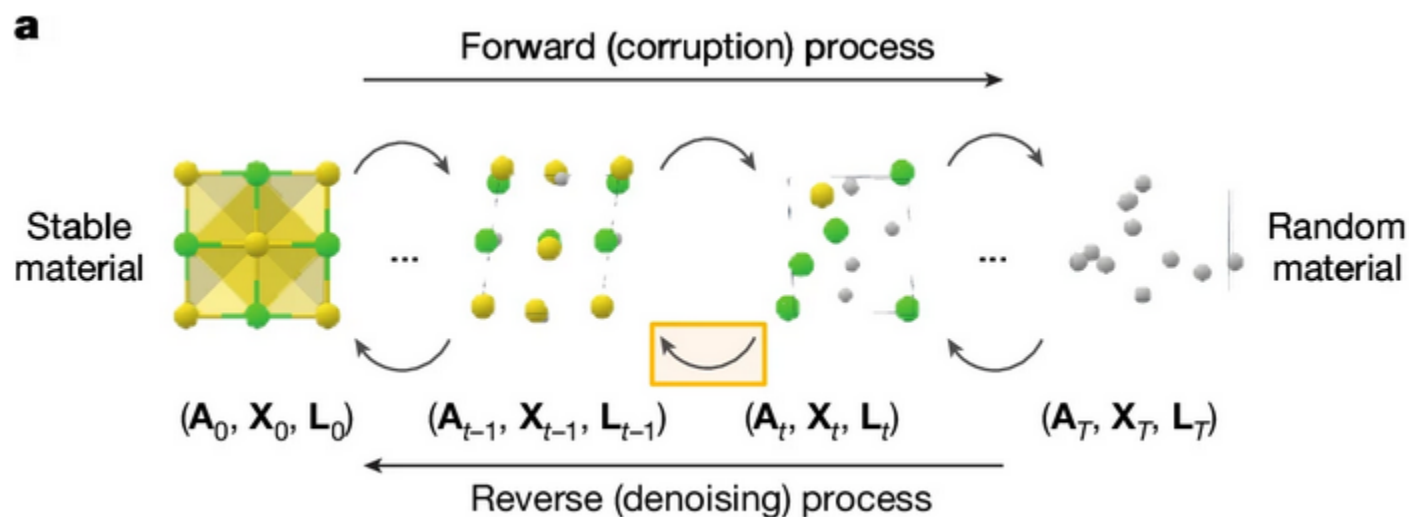


Pretraživanje materijala vs dizajn





Dizajn materijala u AI doba (

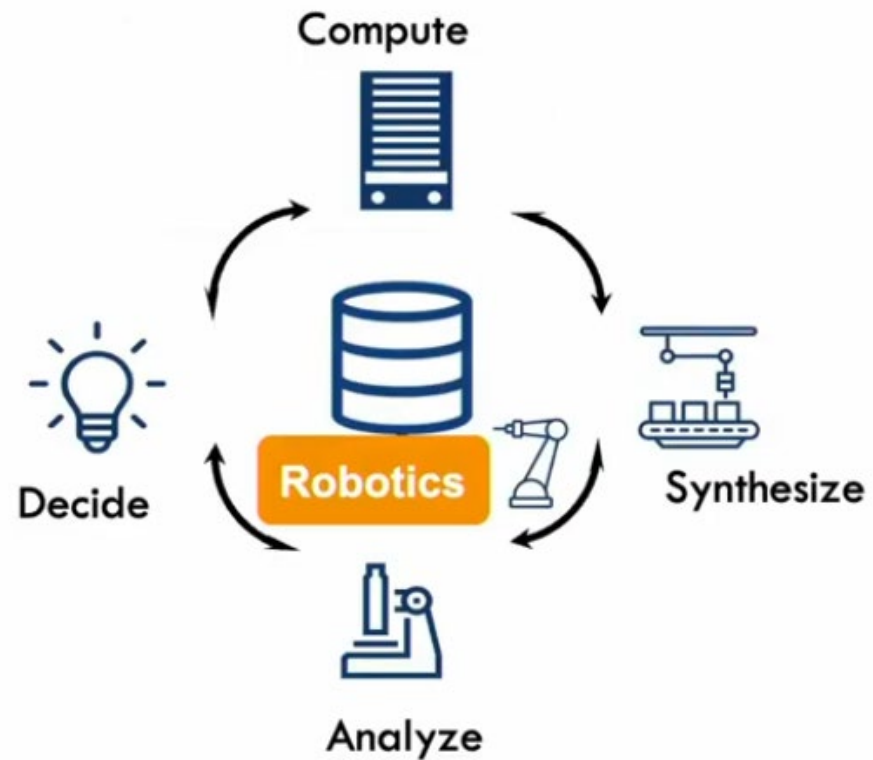


<https://stases.github.io/blogposts/crystalite/>

<https://doi.org/10.1038/s41586-025-08628-5>



Budućnost dizajna materijala





Slijedeći revolucionarni materijal će znanstvenici dizajnirati na (super) računalu uz pomoć umjetne inteligencije?



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