



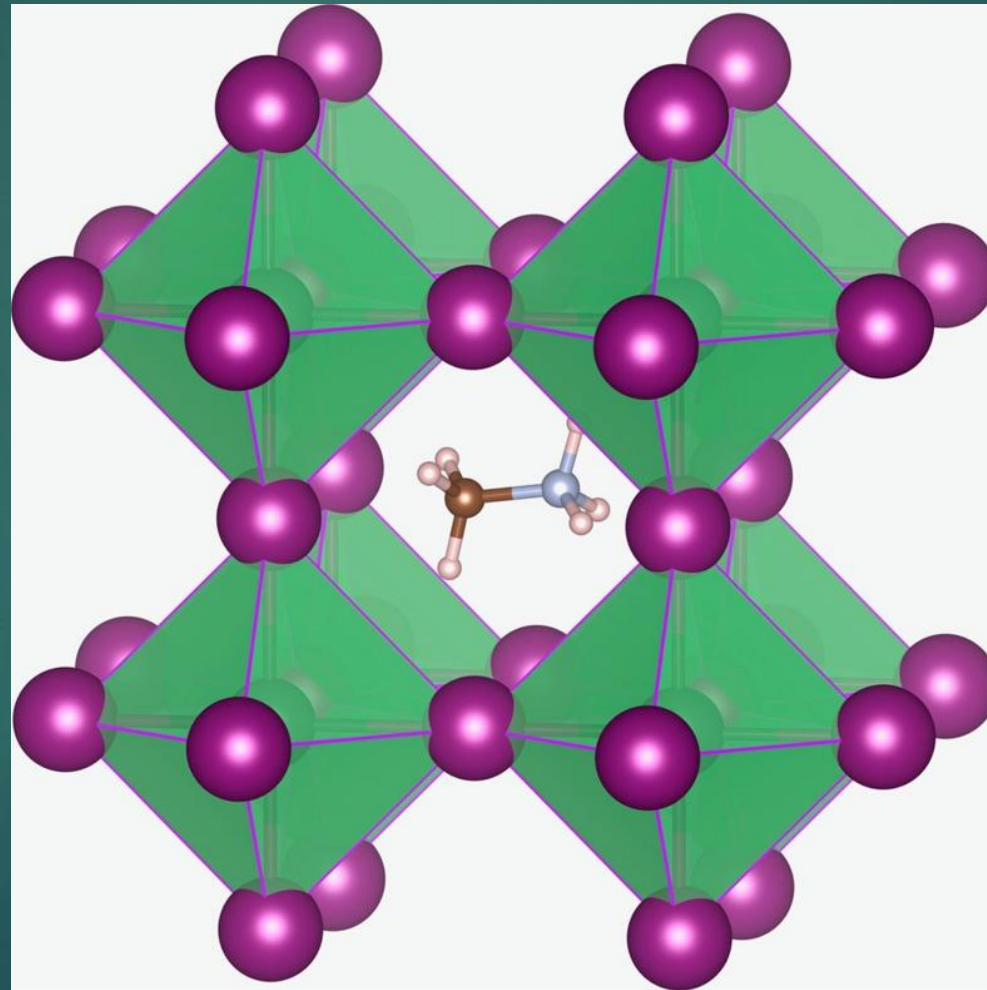
Stabilnost dvodimenzionalnih perovskita

DINO ĐUDARIĆ

MENTOR: LUCA GRISANTI

3D perovskit - MAPbI_3

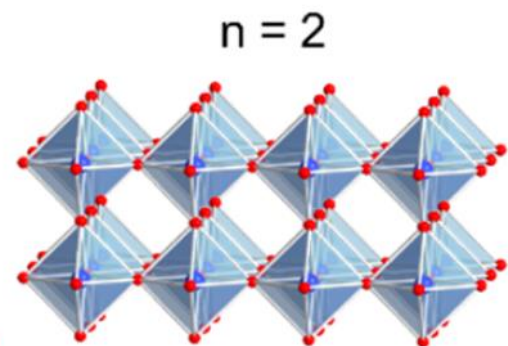
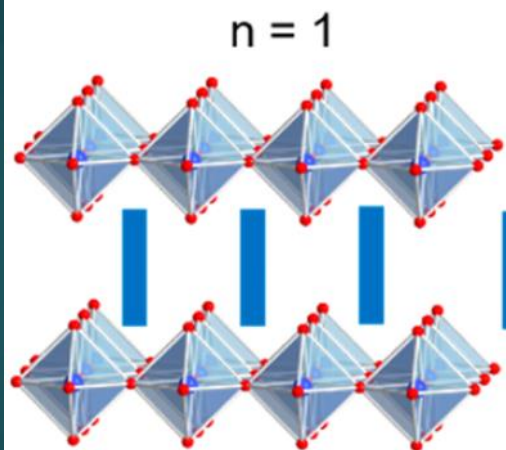
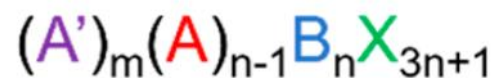
2



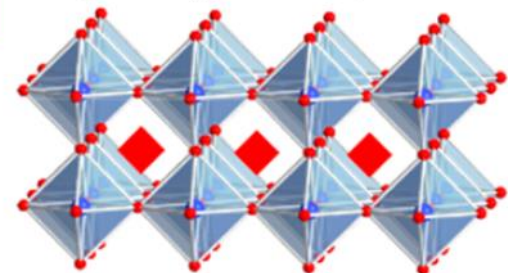
2D perovskite

3

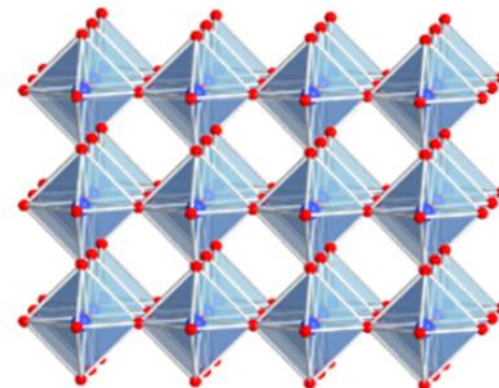
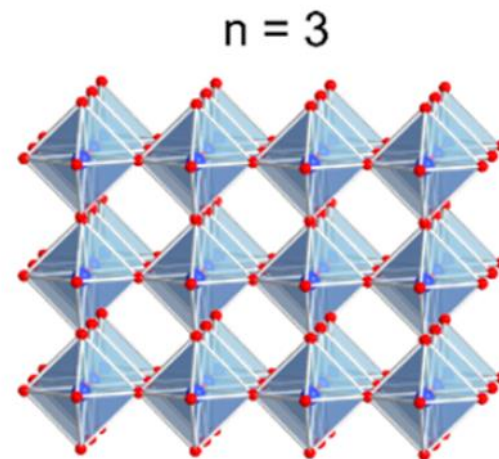
2D Perovskite



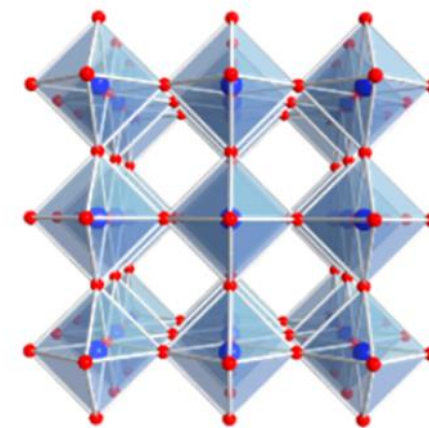
Large organic spacer A'



◆ Small organic cation A
(A = Cs⁺, MA⁺ or FA⁺)



3D Perovskite



B metal, Pb²⁺, Sn²⁺, Ge²⁺
X halide, Cl⁻, Br⁻, I⁻

Teorija funkcionala gustoće (DFT)

- ▶ P. Hohenberg i W. Kohn, Inhomogeneous Electron Gas, Phys.Rev. 136 (1064) B864–B871.
- ▶ W. Kohn i L.J. Sham, Self-Consistent Equations Including Exchange and Correlation Effects, Phys.Rev. 140 (1965) A1133–A1138.

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + U(\vec{r}) + V_H(\vec{r}) \right] \psi_m(\vec{r}) + \int d\vec{r}' V_{xc}(\vec{r}', \vec{r}) \psi_m(\vec{r}') = e_m \psi_m(\vec{r})$$

$$n(\vec{r}) = \sum_{\text{popunjena stanja}} |\psi_n(\vec{r})|^2$$

Quantum espresso

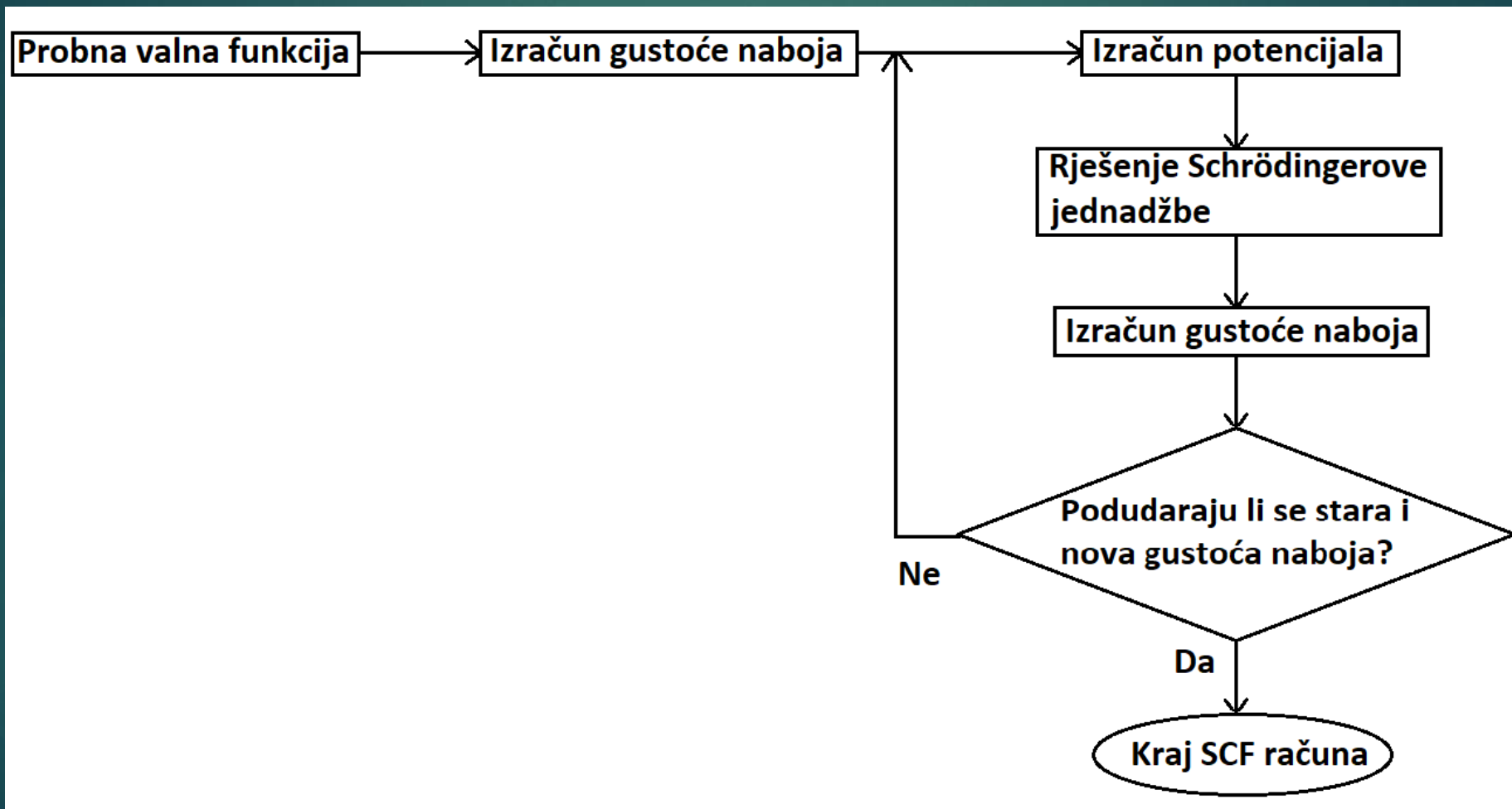
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- ▶ Baza - ravni valovi
- ▶ Pseudopotencijali
- ▶ SCF – samosuglasno polje
- ▶ 'relax' i 'vc-relax' rutine (BFGS algoritam)
- ▶ 'vdW-DF-cx' - van der Waals funkcional gustoće s konzistentnom izmjenom



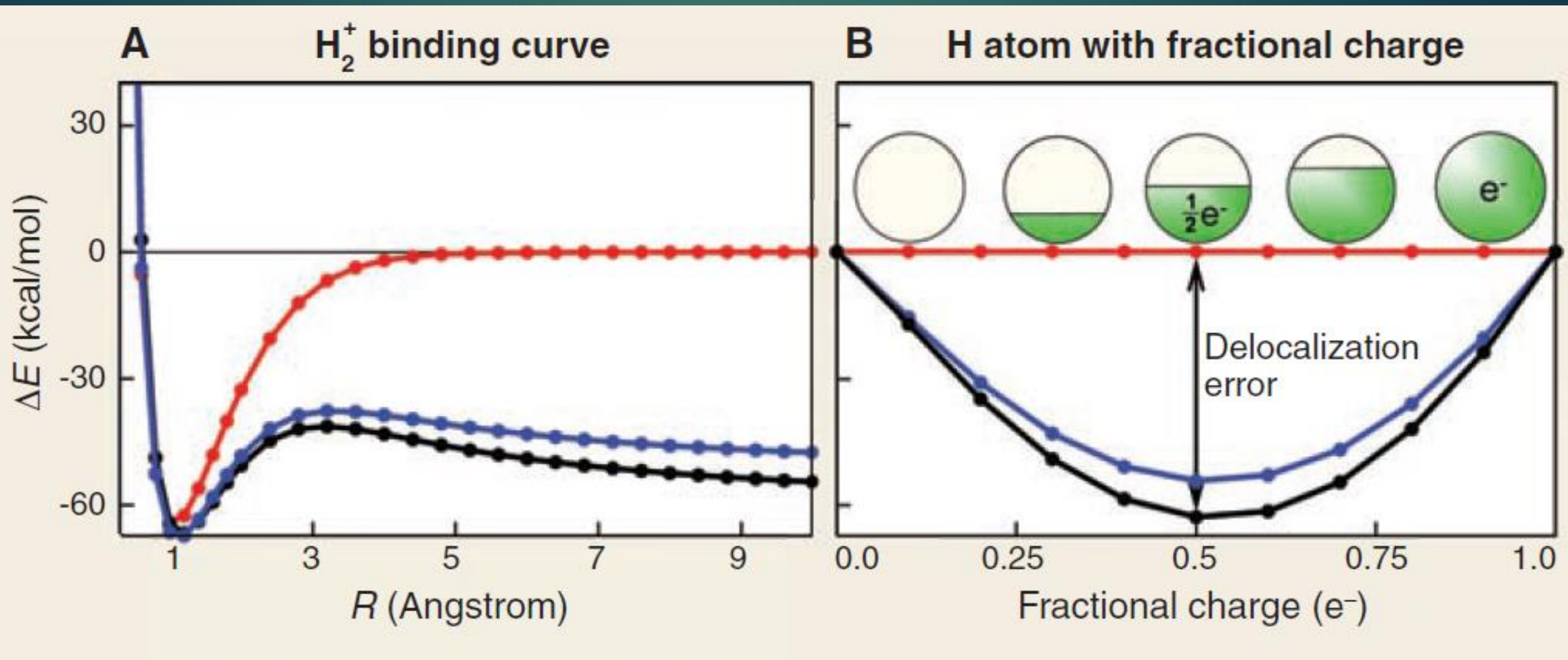
SCF - samosuglasno polje

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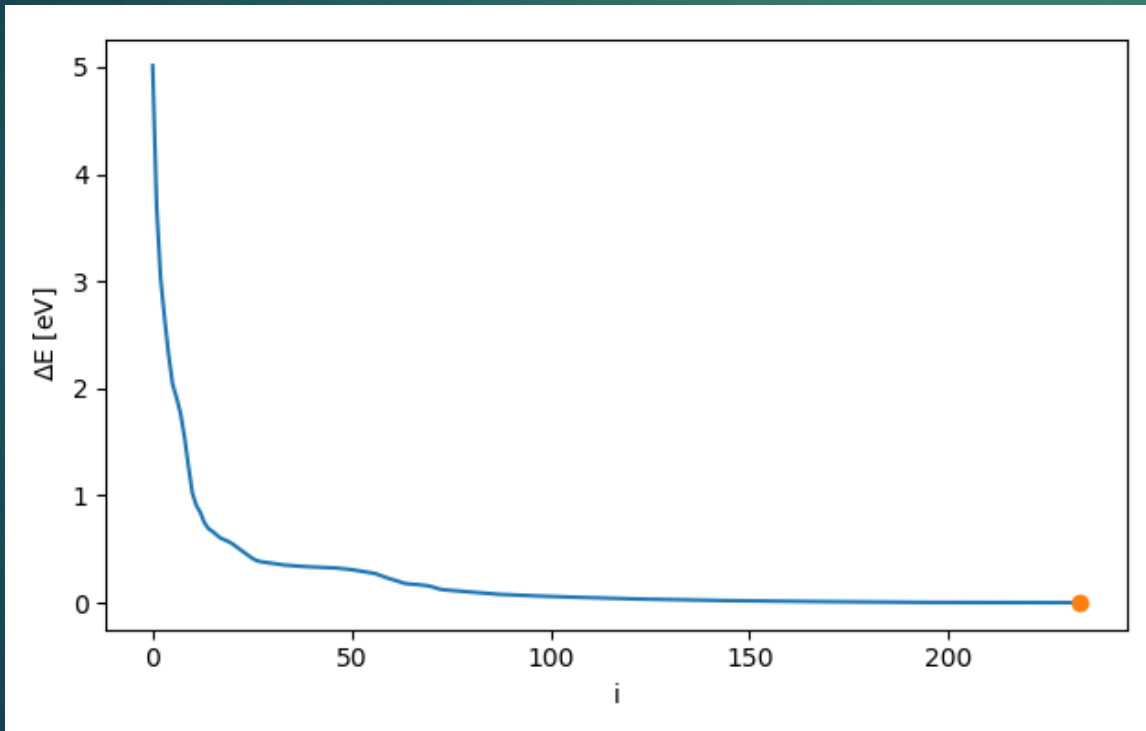
Delokalizacijska pogreška

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Izračun reakcijske energije

$$E_R = \sum_{\text{produkti}} E - \sum_{\text{reaktanti}} E$$



Relaksacija MAPbI₃

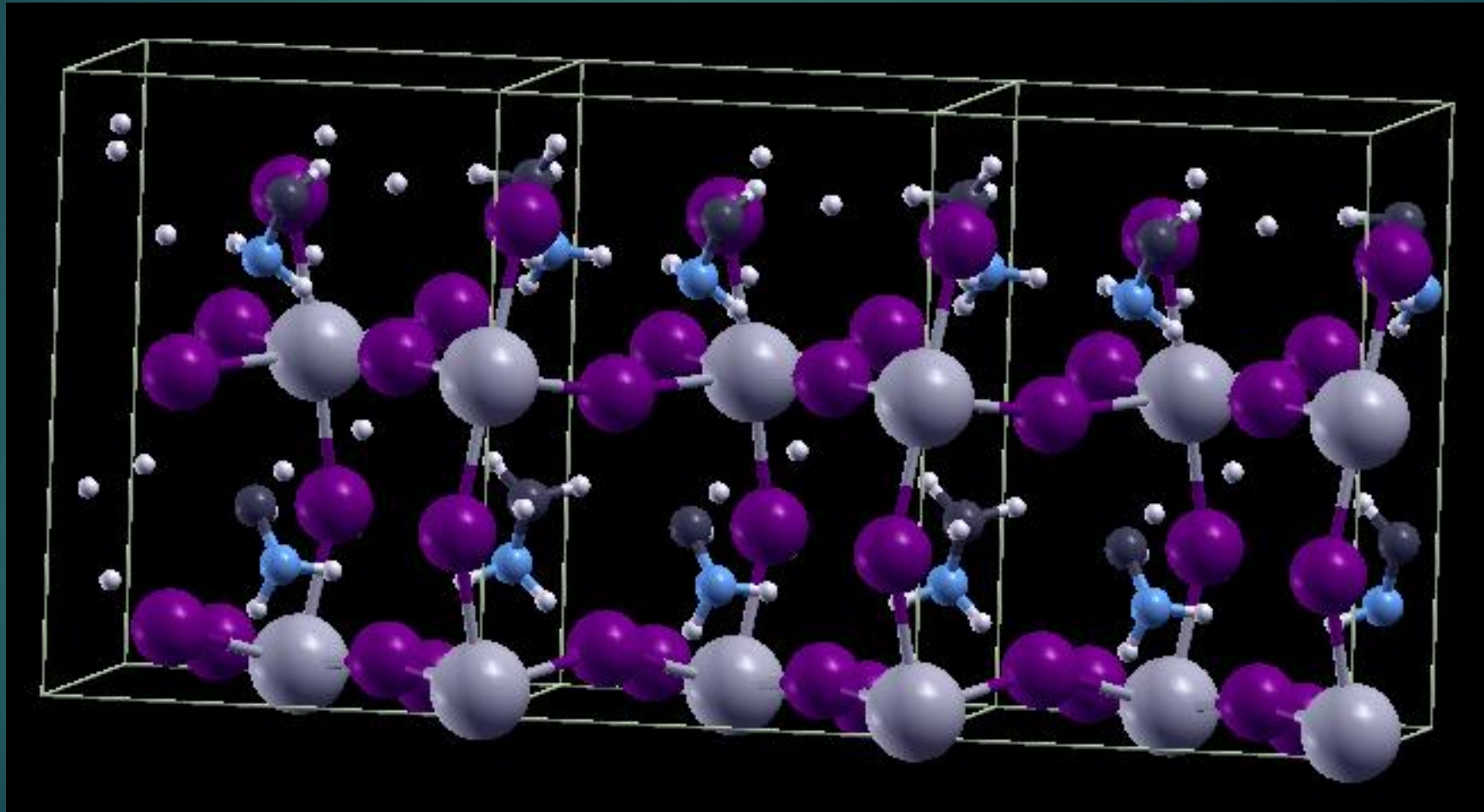
Rezultati: 3D perovskit + O₂



	Izračunato E _R	Literatura E _R
MAPbI ₃	4.60 eV	1.56 eV
MAPbBr ₃	7.08 eV	4.98 eV

Relaksirana struktura MAPbI_3

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Rezultati: 3D perovskit + O₂⁻

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	Izračunato E _R	Literatura E _R
MAPbI ₃	7.36 eV	-1.39 eV
MAPbBr ₃	9.88 eV	2.00 eV

Rezultati: 2D perovskit + O₂

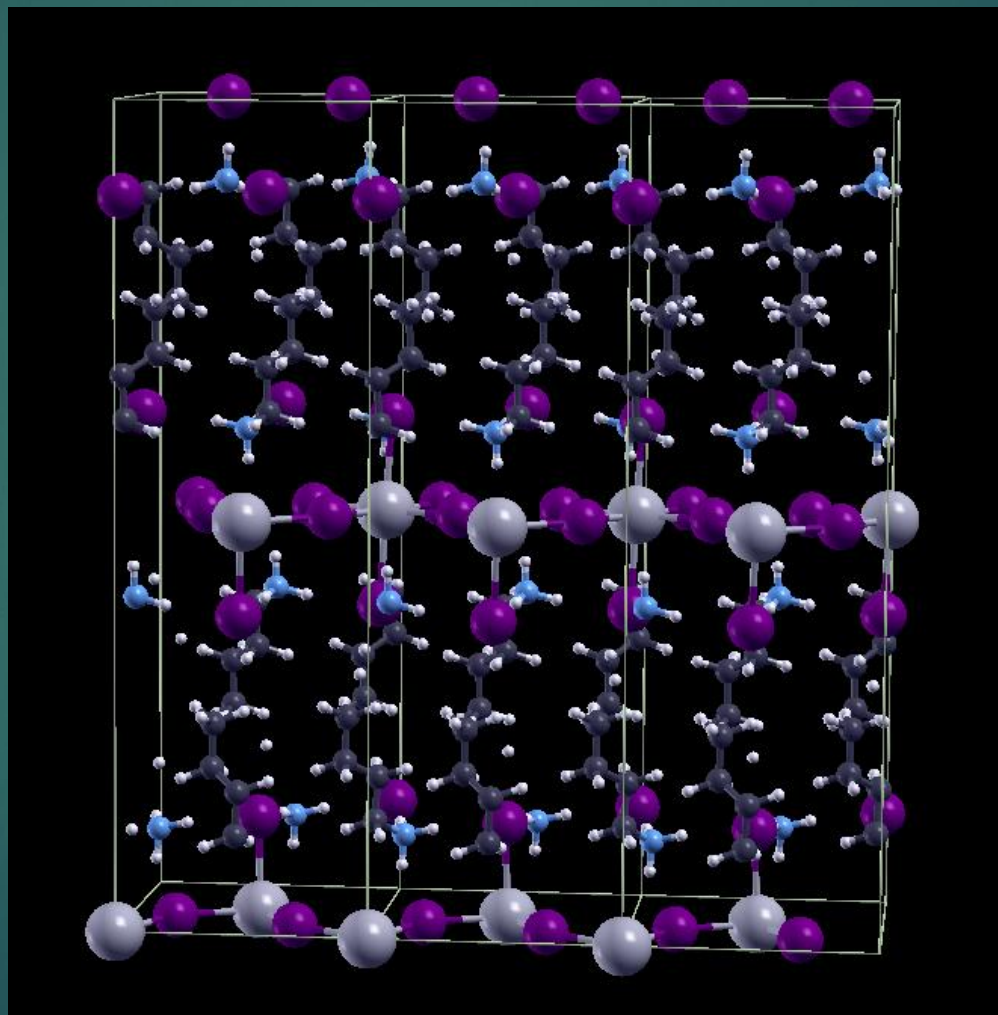
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	Izračunato E _R	Razlika u odnosu na 3D
(BAH) ₂ PbI ₄	5.83 eV	1.23 eV
(BAH) ₂ PbBr ₄	8.07 eV	0.99 eV

Relaksirana struktura $(\text{BAH})_2\text{PbI}_4$

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Zaključak

- ▶ Reakcijska energija 3D perovskita s kisikom
- ▶ Reakcijska energija 3D perovskita sa superoksidom
- ▶ Reakcijska energija 2D perovskita s kisikom
- ▶ Preporučeni budući izračuni reakcijskih energija 3D i 2D perovskita s kisikom i superoksidom u strukturi perovskita

- ▶ Chem. Mater. 2020, 32, 1, 400–409
- ▶ Eames C, Frost JM, Barnes PR, O'Regan BC, Walsh A, Islam MS. Ionic transport in hybrid lead iodide perovskite solar cells. Nat Commun. 2015 Jun 24;6:7497.
- ▶ J. Am. Chem. Soc. 2019, 141, 1171-1190
- ▶ A. J. Cohen, P. Mori-Sanchez, W. Yang, Science 321, 792 (2008).

HVALA NA PAŽNJI