MODELOVANJE
- PRIMENA I INTERDISCIPLINARNOST -

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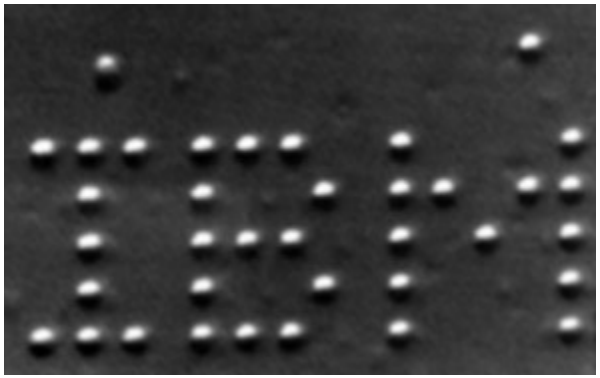
Departman za fiziku

www.armakovic.com

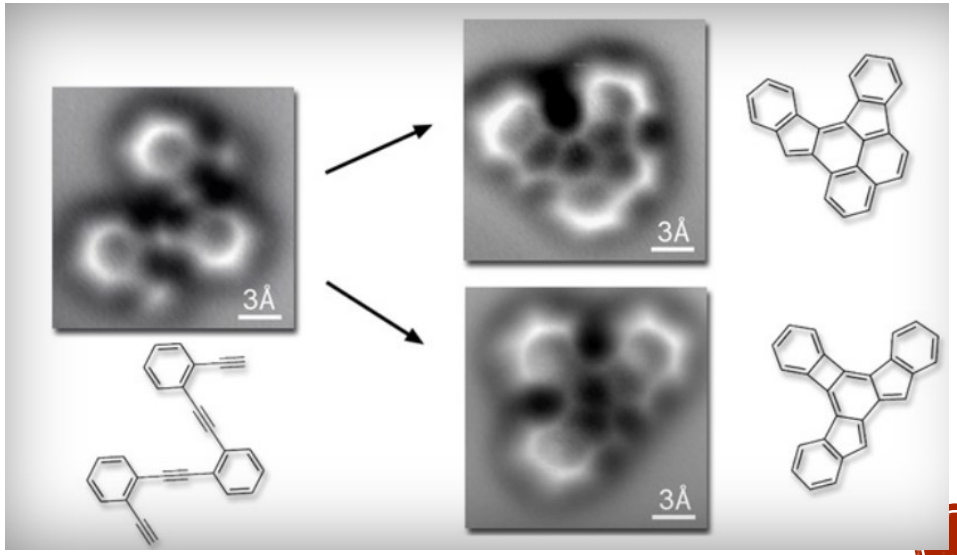
DA LI SE ATOMI I MOLEKULI MOGU „VIDETI“?

1989.

- Atomi Xe na površini Ni
- Scanning tunneling microscope
- Donald Eigler and Erhard Schweizer



Lawrence Berkeley National Laboratory



2013.

- University of Victoria
- Težina: 7 tona
- Cena: ~30 M $
- Rezolucija: 35 pm

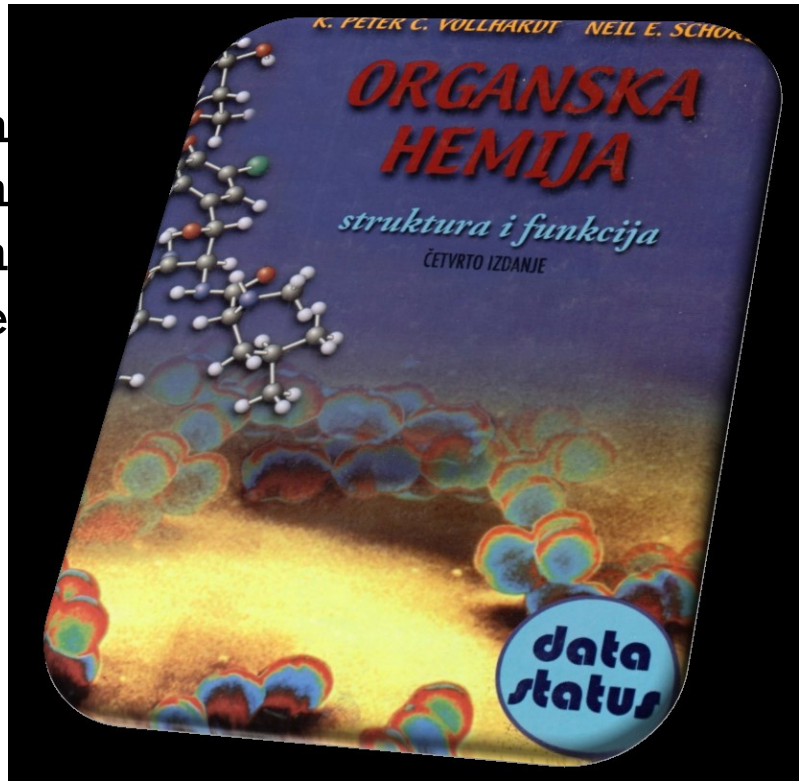
THE FIRST IMAGE OF BLACK HOLE!?!

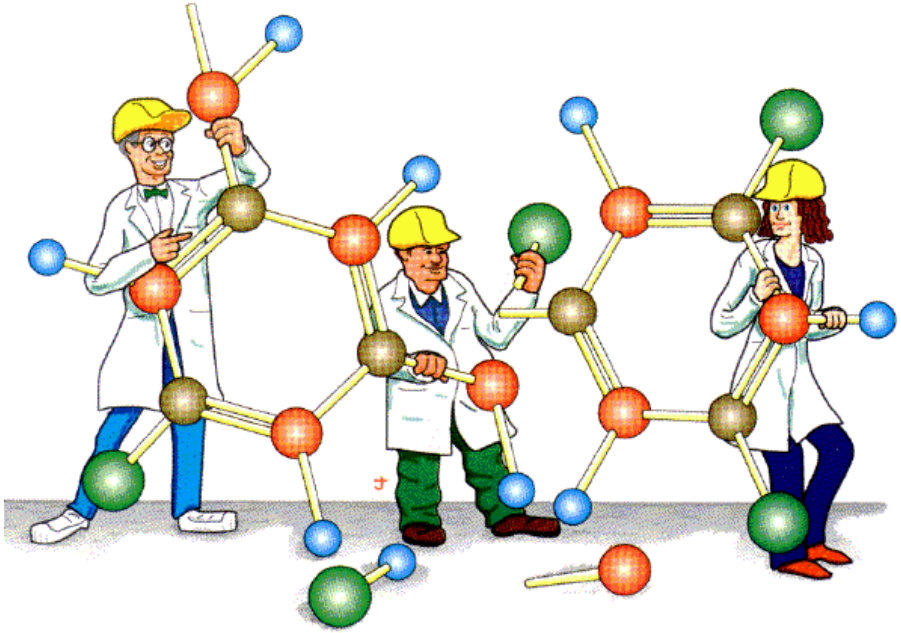
E SAD PRAVE SLIKE!

I DALJE JE OSLONAC (MOLEKULSKO) MODELOVANJE

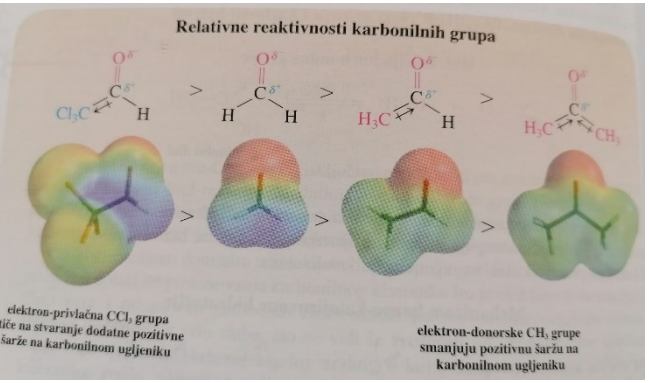
Definicija:

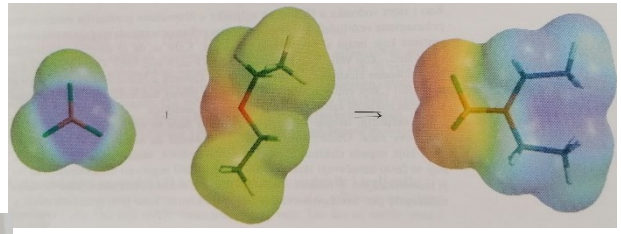
Molekulsko modelovanje predstavlja povezivanje teorijskih i kompjuterskih resursa radi dobijanja relevantnih informacija o fenomenima koji se odvijaju na molekulskom nivou

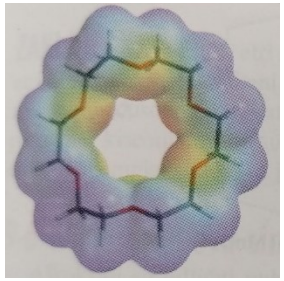


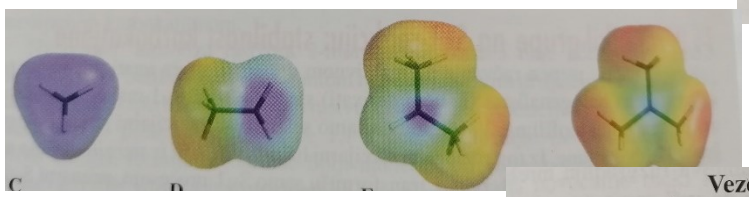


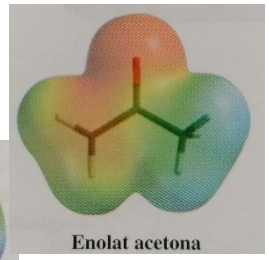
"THE FIRST CONTACT" SA MODELOVANJEM - WOLLHARDT -

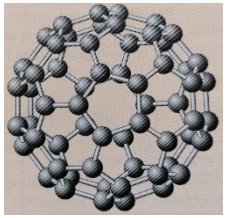


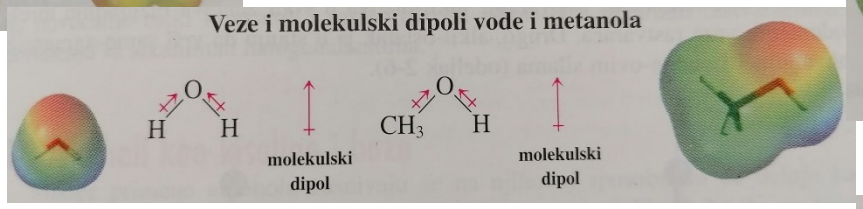


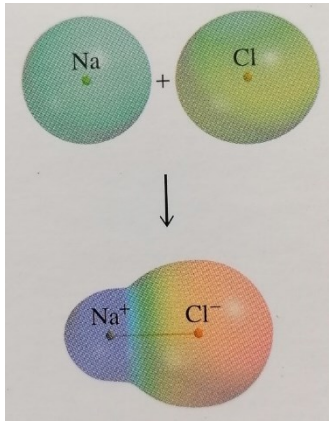


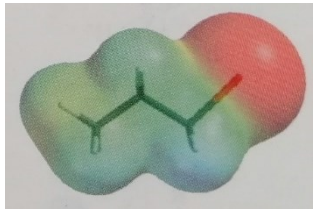


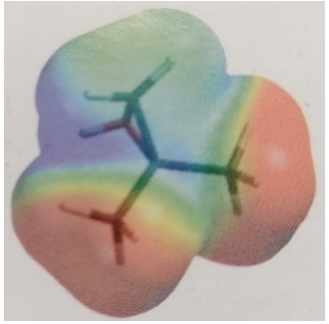


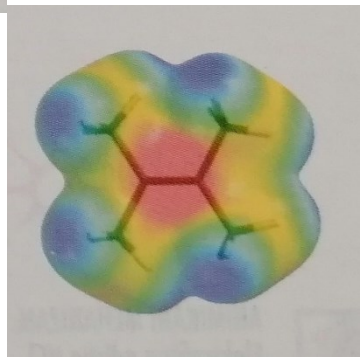










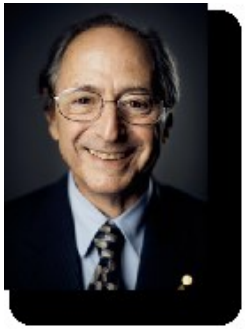


NOBELOVE NAGRADE

2013. Nobel Prize in Chemistry

"For the development of multiscale models for complex chemical systems"

Martin Karplus



Michael Levitt

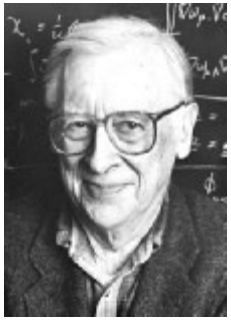
Arieh Warshel

1998. Nobel Prize in Chemistry

Kohn: "For his development of the density-functional theory"

Pople: "for his development of computational methods in quantum chemistry"

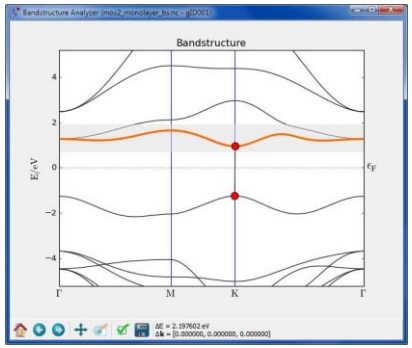
Walter Kohn

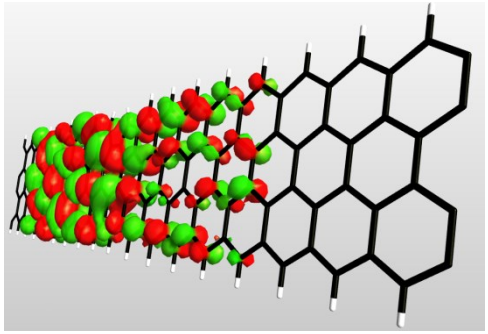


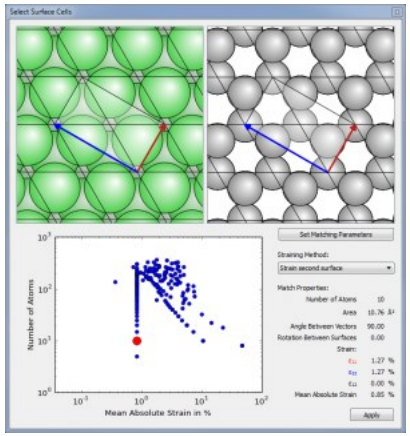
John Pople

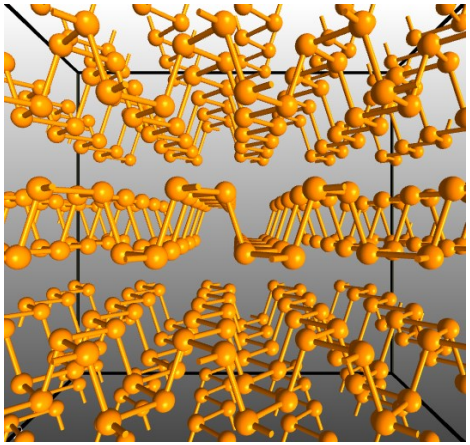
VIRTUAL NANOLAB ATOMISTIX TOOLKIT

www.quantumwise.com









Moćan alat za istraživanje:

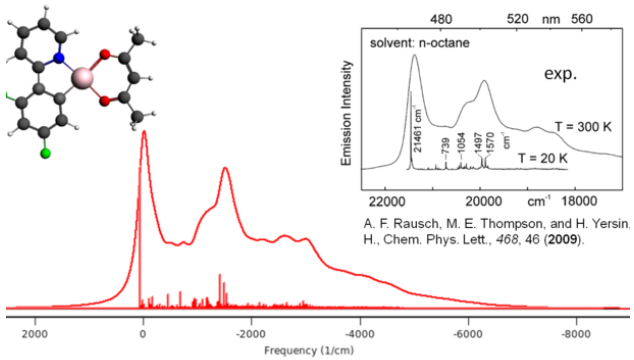
- Izolovanih molekula,
- Periodičnih nanostruktura
- Površi
- Uticaja električnog polja
- Transportnih svojstava
- Spintronik svojstava
- Dinamičkih svojstava

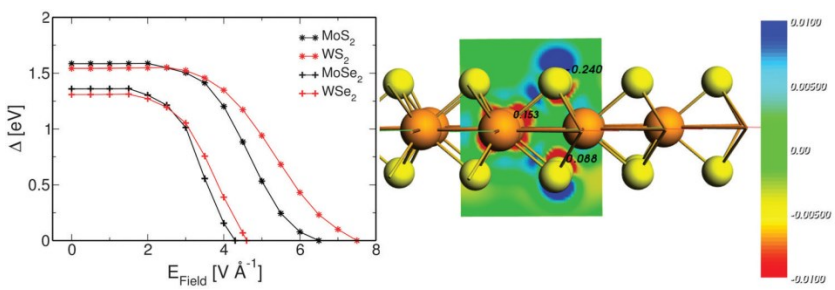
...

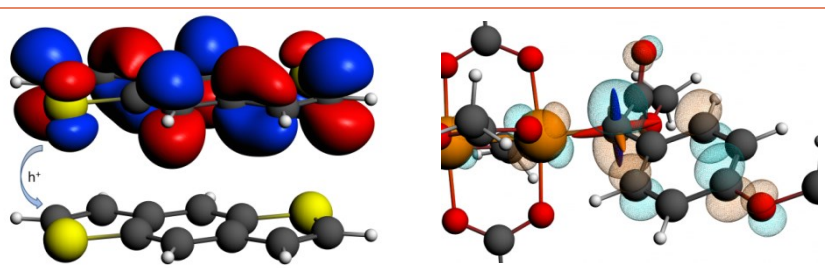
Preko 1000 naučnih radova je napravljeno upotrebom ovog alata

AMSTERDAM DENSITY FUNCTIONAL THEORY MOLECULAR MODELING SUITE

www.scm.com







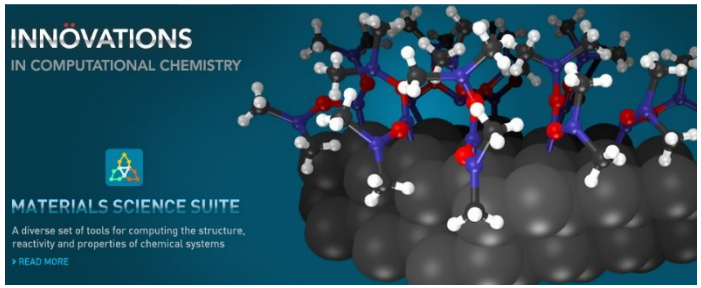
Moćan alat za istraživanje:

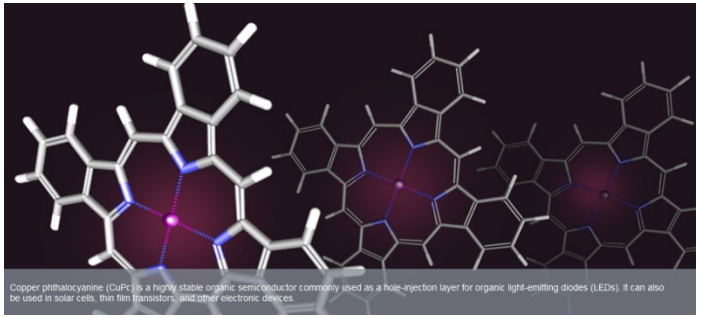
- Izolovanih molekula,
- Periodičnih nanostruktura
- Površi
- Uticaja električnog polja
- Transportnih svojstava
- Reaktivne molekulske dinamike
- Spektroskopije

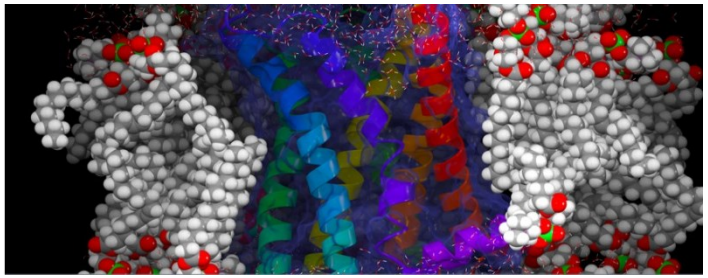
Akcenat na izolovanim molekulima

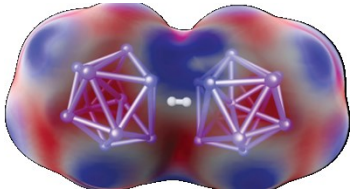
A KORISTIMO JOŠ I SCHRÖDINGER MATERIAL SCIENCE SUITE

MATERIALS SCIENCE SUITE









- Superiorno programsko okruženje kada se radi o performansama i mogućnostima u slučaju izolovanih molekula
- Podrška i za DFT i za MD pristup
- Primena u farmaceutskoj industriji

BESPLATNI ALATI

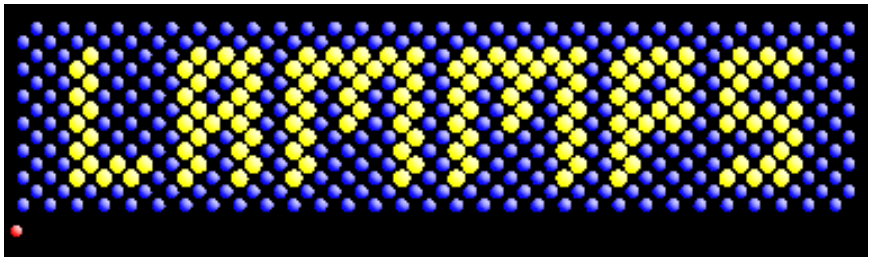
GAMESS

MOPAC®

NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

QUANTUMESPRESSO

abinit



DFTB

MOLEKULSKO MODELOVANJE NA DELU

Koji pristupi

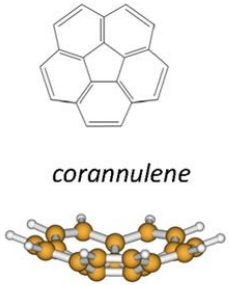
Teorija funkcionala gustine (DFT) i Simulacije molekulske dinamike

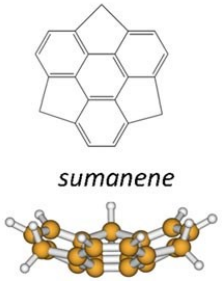
Koja svojstva

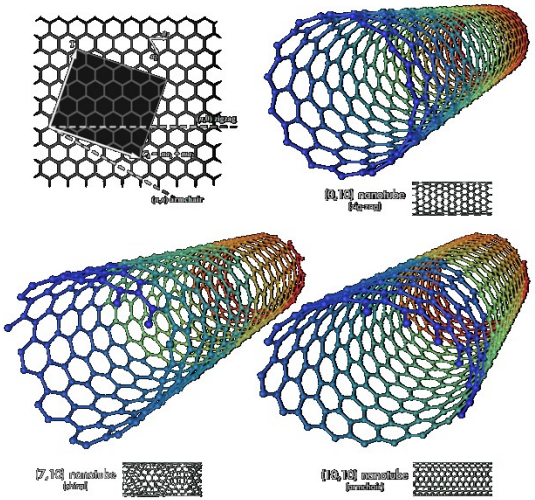
Reaktivna transportna optička adsorpciona

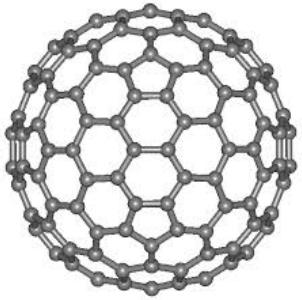
Koje strukture

Farmaceutski molekuli, sumanen, viši aceni, jonske tečnosti, grafeni, fulereni i nanotube



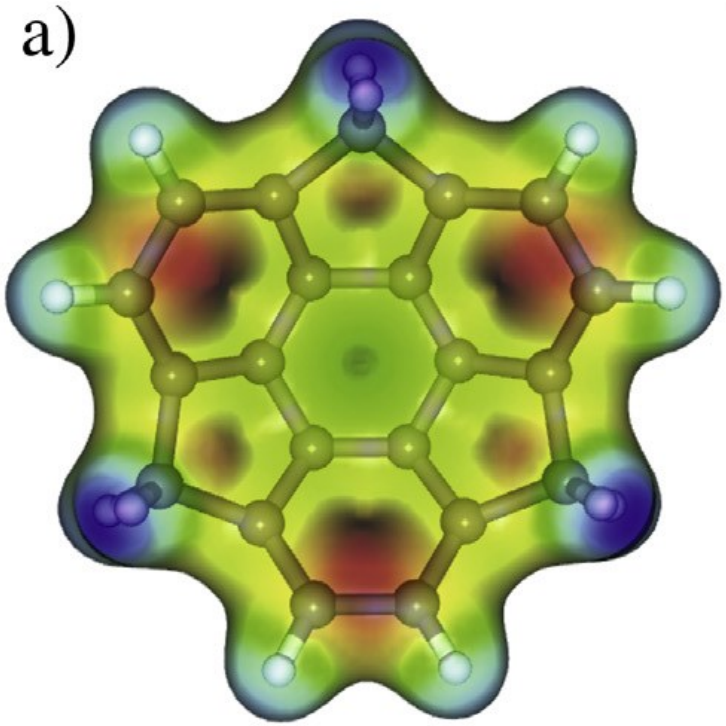


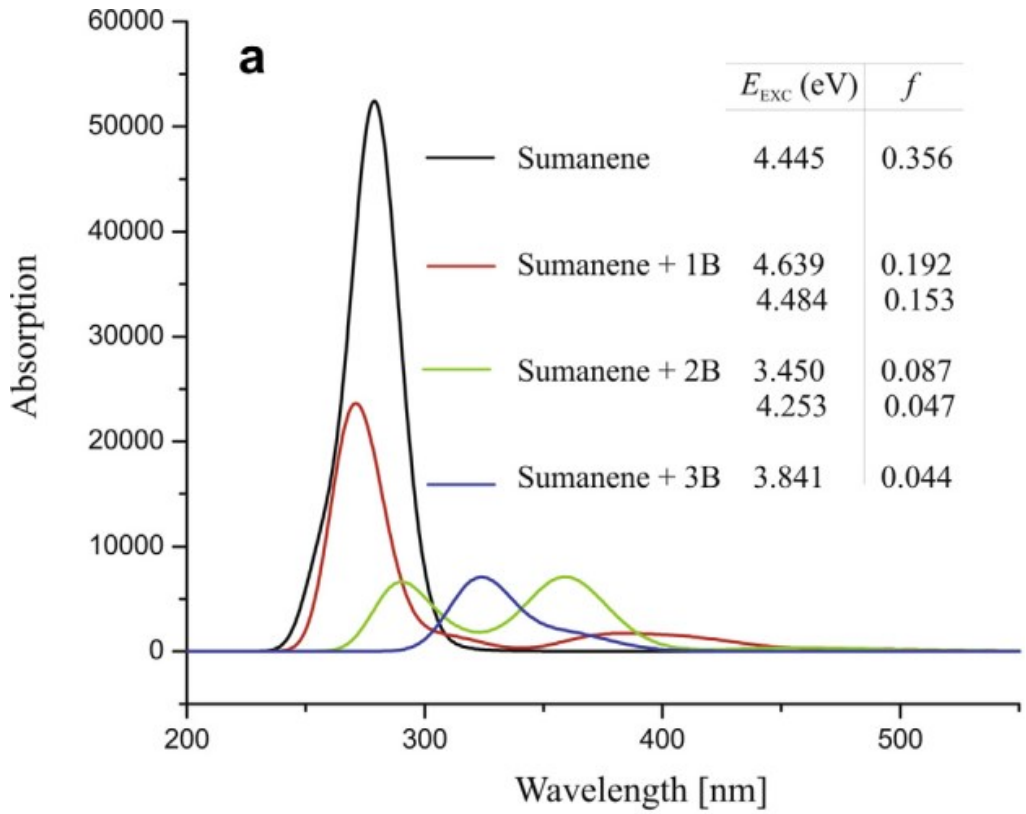




DFT PRORAČUNI

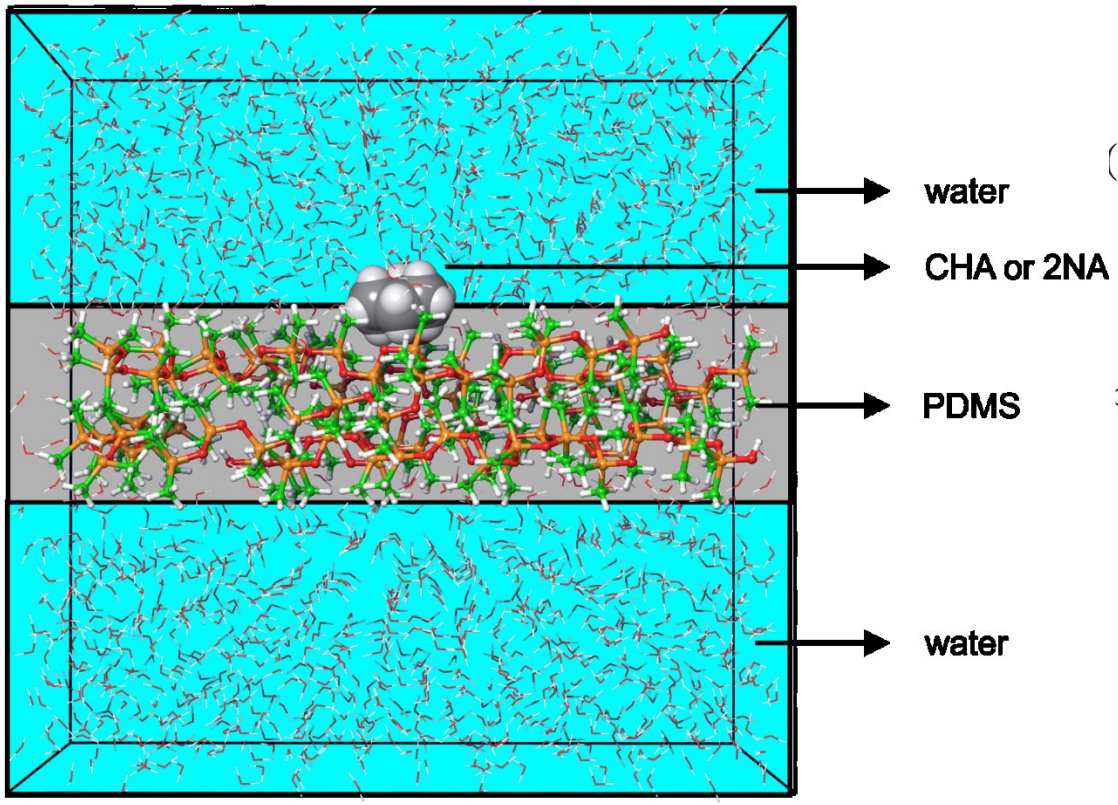
DFT proračuni nam daju informacije kao što su raspodela naelektrisanja, molekulski elektrostatički potencijal, srednje lokalne energije jonizacije, indekse reaktivnosti, spektre, itd.

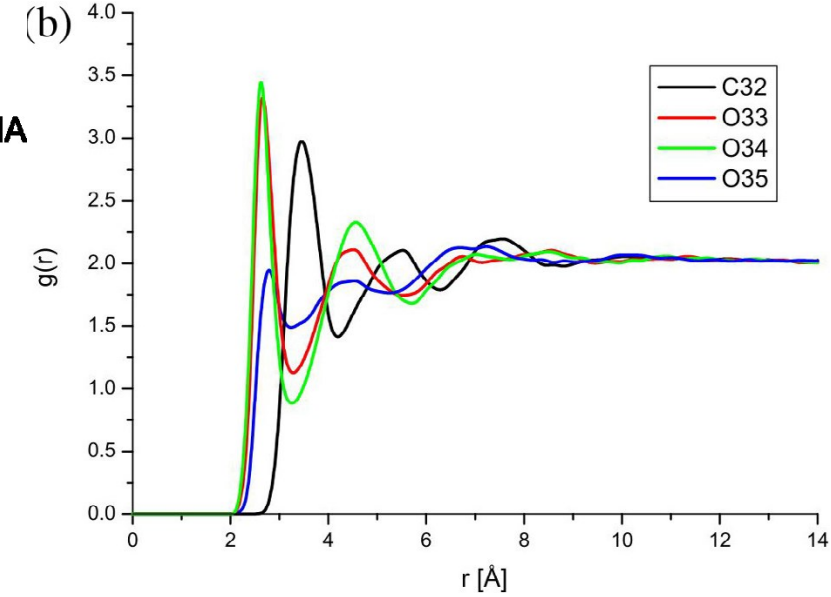




SIMULACIJE MOLEKULSKE DINAMIKE

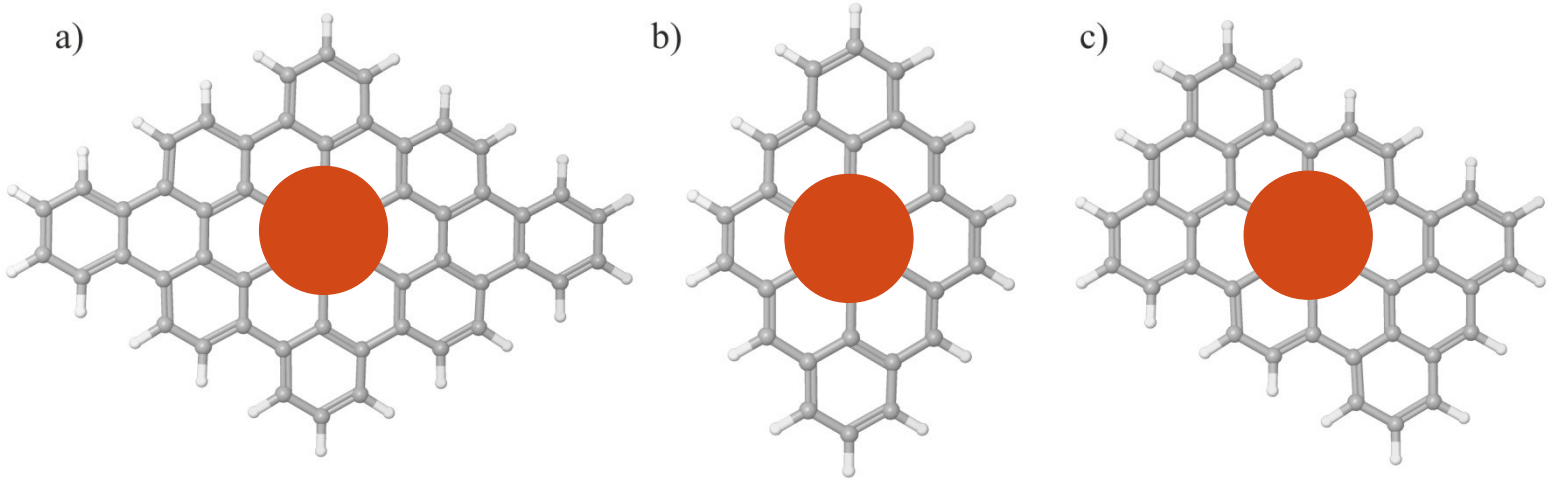
Simulacije molekulske dinamike nam daju informacije o interakciji molekula sa rastvaračima, posebno sa molekulima vode, preko tzv. radijalnih distributivnih funkcija (RDF) čiji nam profili ukazuju na „gomilanje “ molekula rastvarača oko atoma molekula.





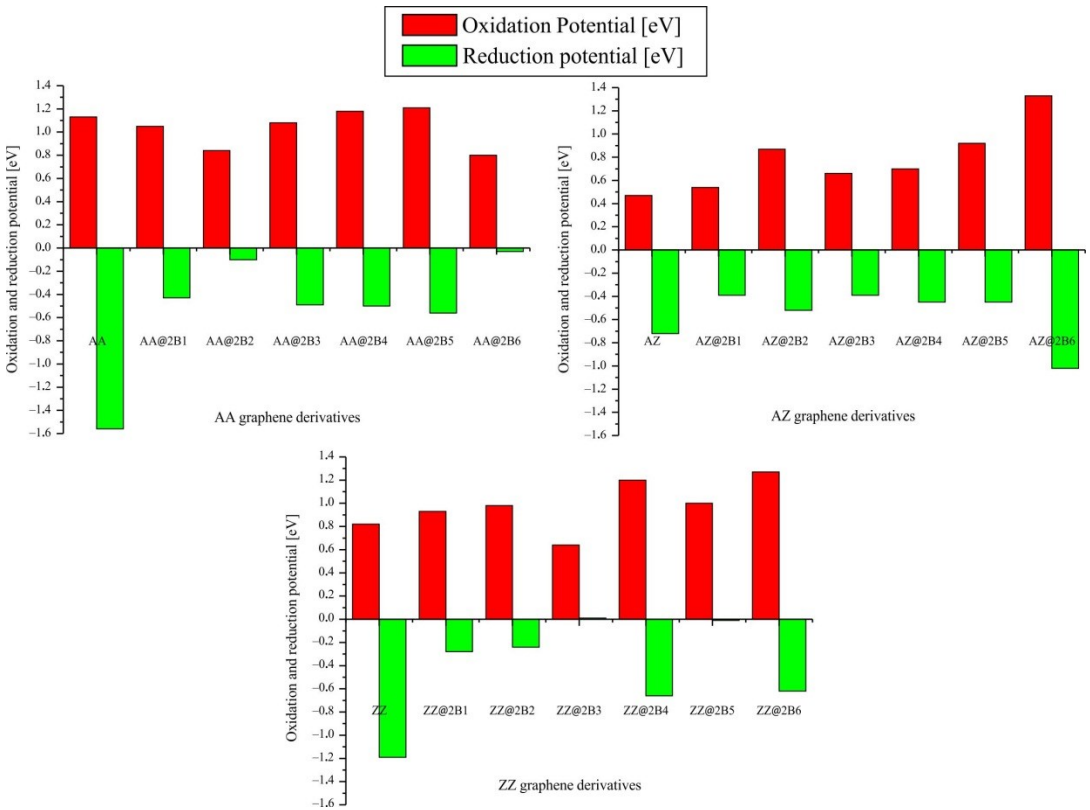
OPTOELEKTRONSKA I TRANSPORTNA SVOJSTVA GRAFENA

Ispitivanje uticaja dopiranja atomima bora



Centralni prsteni modela grafenskih nanočestica modifikovani su sa po dva atoma bora. Ukupno dobijeno 18 struktura, koje su dalje podvrgnute ispitivanju optoelektronskih i transportnih svojstava

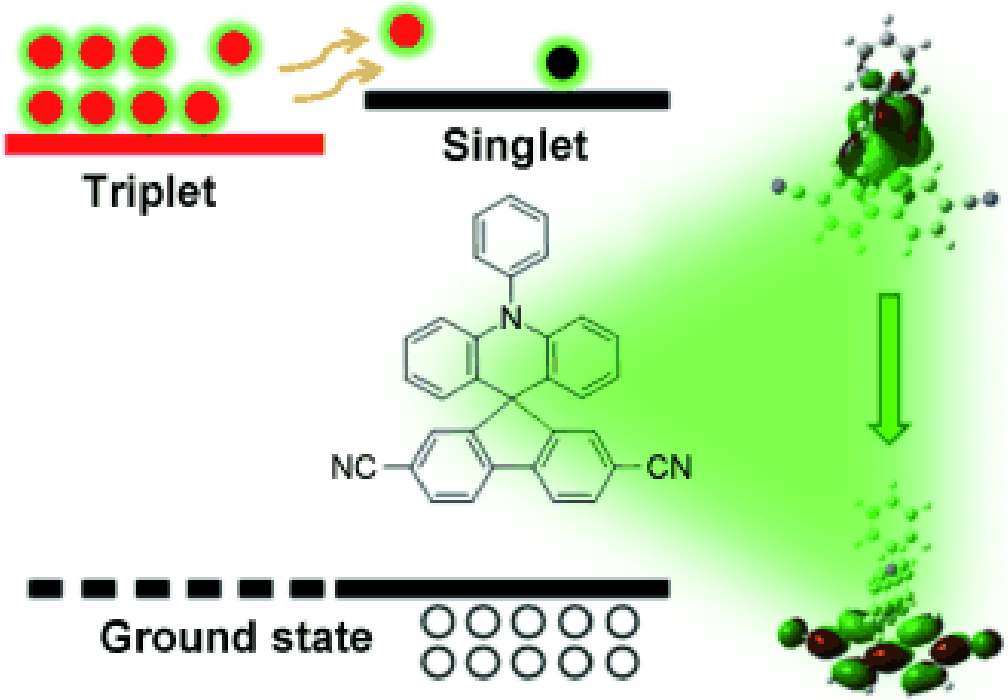
OKSIDACIONI I REDUKCIONI POTENCIJAL



- Oksidacioni i redukcioni potencijal ukazuju na to koliko je neku molekulsku strukturu lako/teško oksidovati
- Bitno za proces „oksidacionog nagrizanja“ (oxidation etching)
- Vidi se da modifikacije atomima bora menjaju oksidacioni i redukcioni potencijal u oba smera, dakle pogodni su i za povećanje i smanjenje reaktivnosti.

TADF MEHANIZAM

TADF je skraćenica od Thermally Activated Delayed Fluorescence



$$\Delta E(S_1 - T_1)$$

Što je niža vrednost ovog parametra, to je potencijal primene molekula kao OLED materijala veća, treba da je **<0.37 eV**

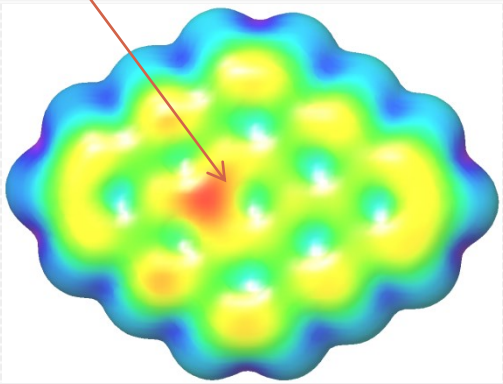
REAKTIVNA SVOJSTVA GRAFENSKIH NANOČESTICA MODIFIKOVANIH SA B, N, Al, Si i P ATOMIMA

ALIE površi

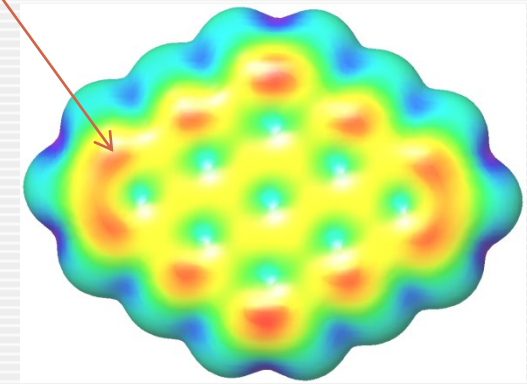
~185 kcal/mol

200 kcal/mol

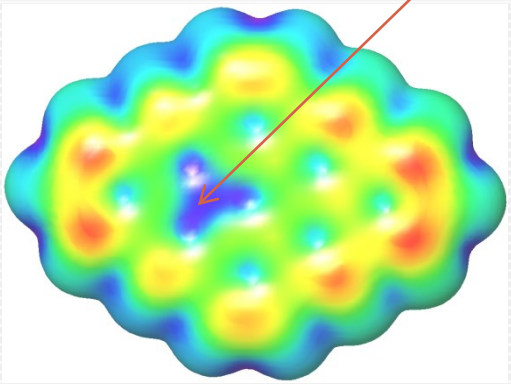
~ 300 kcal/mol



ZZ@B

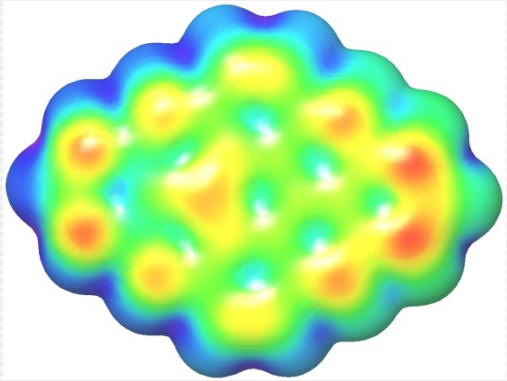


Pristine ZZ model

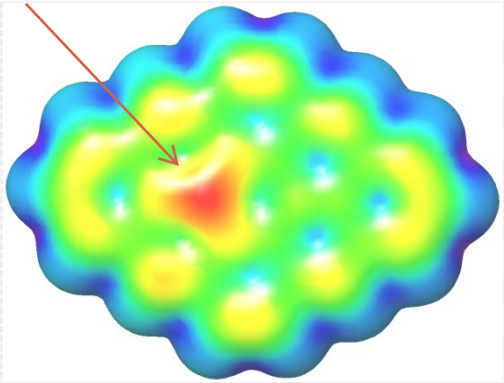


ZZ@N

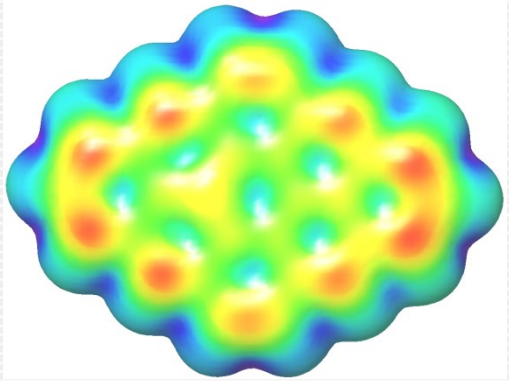
~190 kcal/mol



ZZ@Al



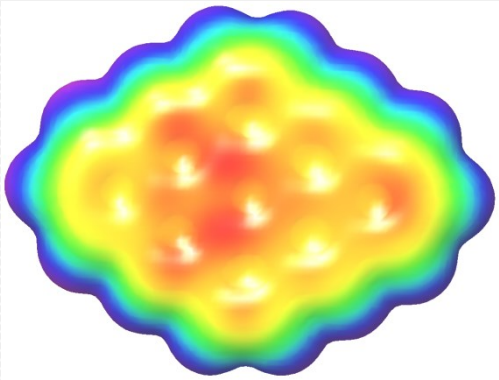
ZZ@Si



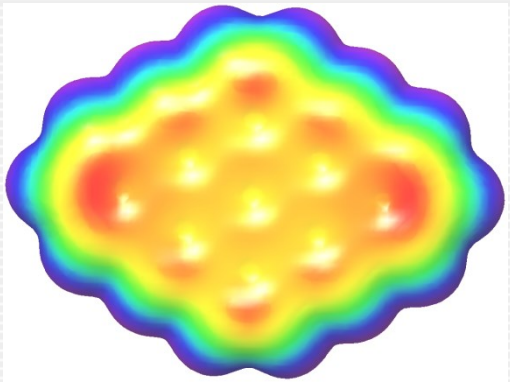
ZZ@P

REAKTIVNA SVOJSTVA GRAFENSKIH NANOČESTICA MODIFIKOVANIH SA B, N, Al, Si i P ATOMIMA

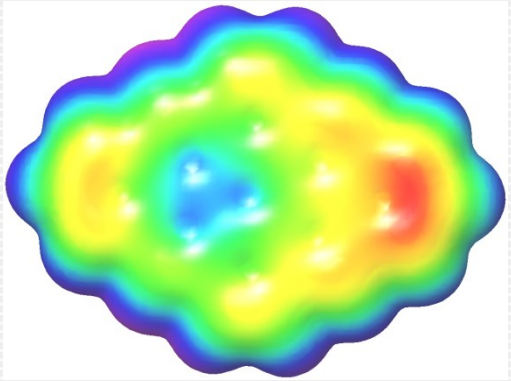
MEP površi



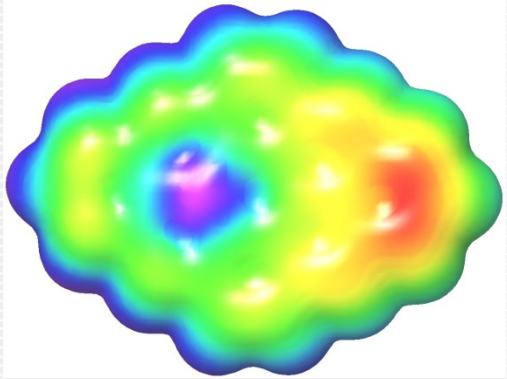
ZZ@B



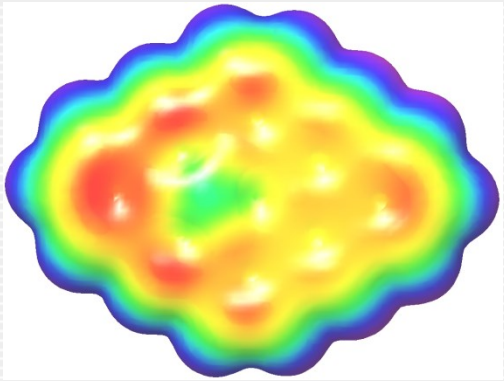
Pristine ZZ model



ZZ@N



ZZ@Al



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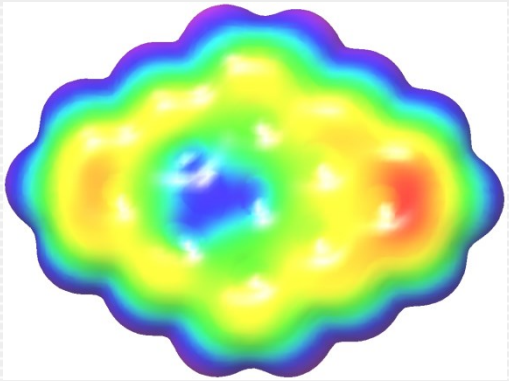

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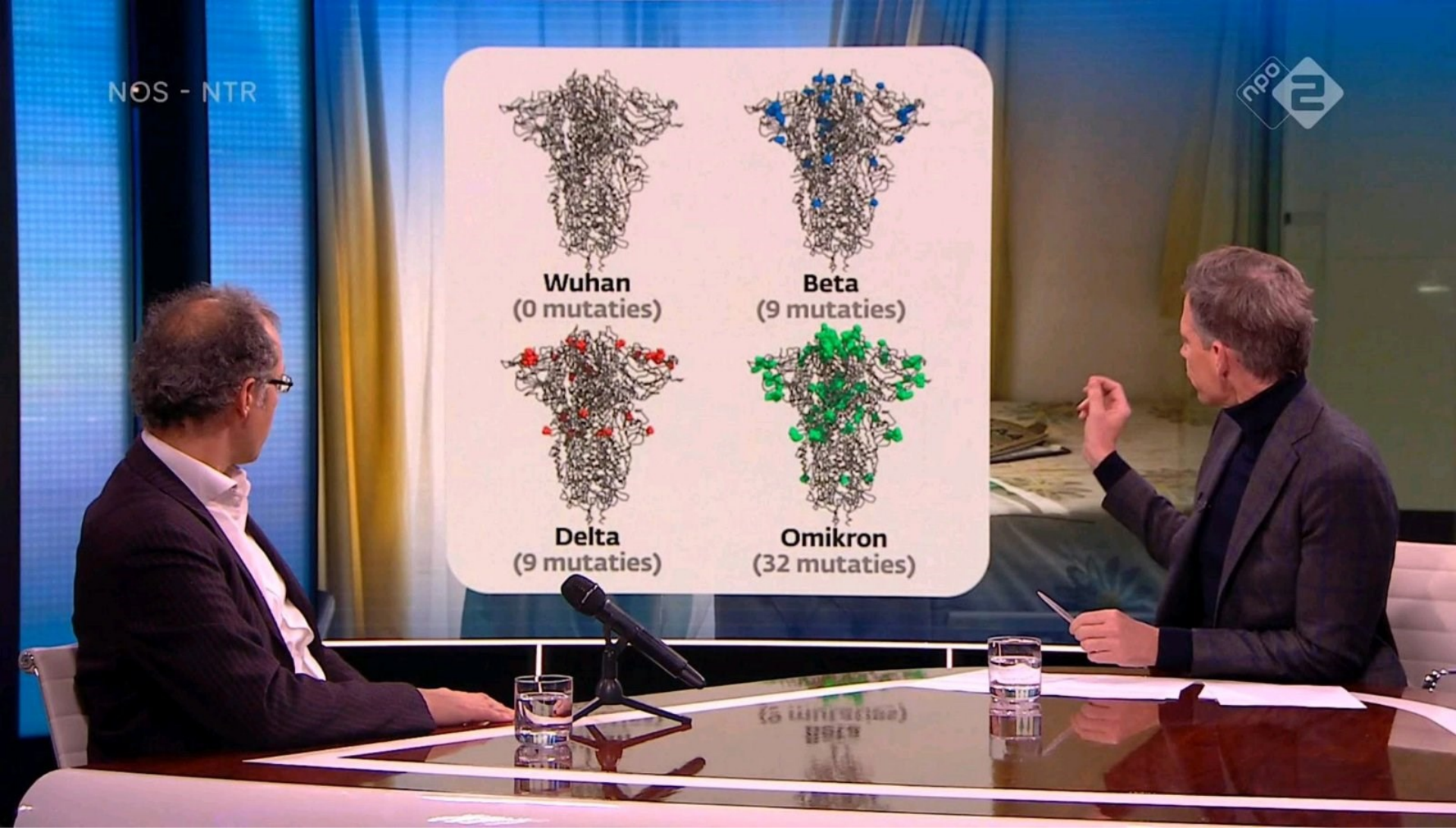

NOS - NTR
npo 2
Wuhan
(0 mutaties)
Beta
(9 mutaties)
Delta
(9 mutaties)
Omikron
(32 mutaties)

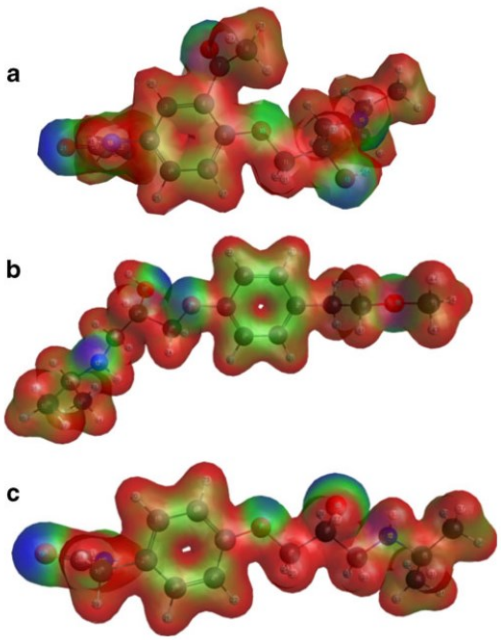
KAKO JE SVE POČELO

- Konferencija mladih istraživača, 2010. godina
- Nedostatak softverskih i kompjuterskih resursa
- Odabir manjih struktura i besplatnih alata (GAMESS i Avogadro)
- Izbor na molekulima lekova

PROŠLA DECENIJA ☺

J Mol Model (2012) 18:4491–4501
DOI 10.1007/s00894-012-1457-5

ORIGINAL PAPER



Active components of frequently used β-blockers from the aspect of computational study

Stevan Armaković · Sanja J. Armaković · Jovan P. Šetrajčić · Igor J. Šetrajčić

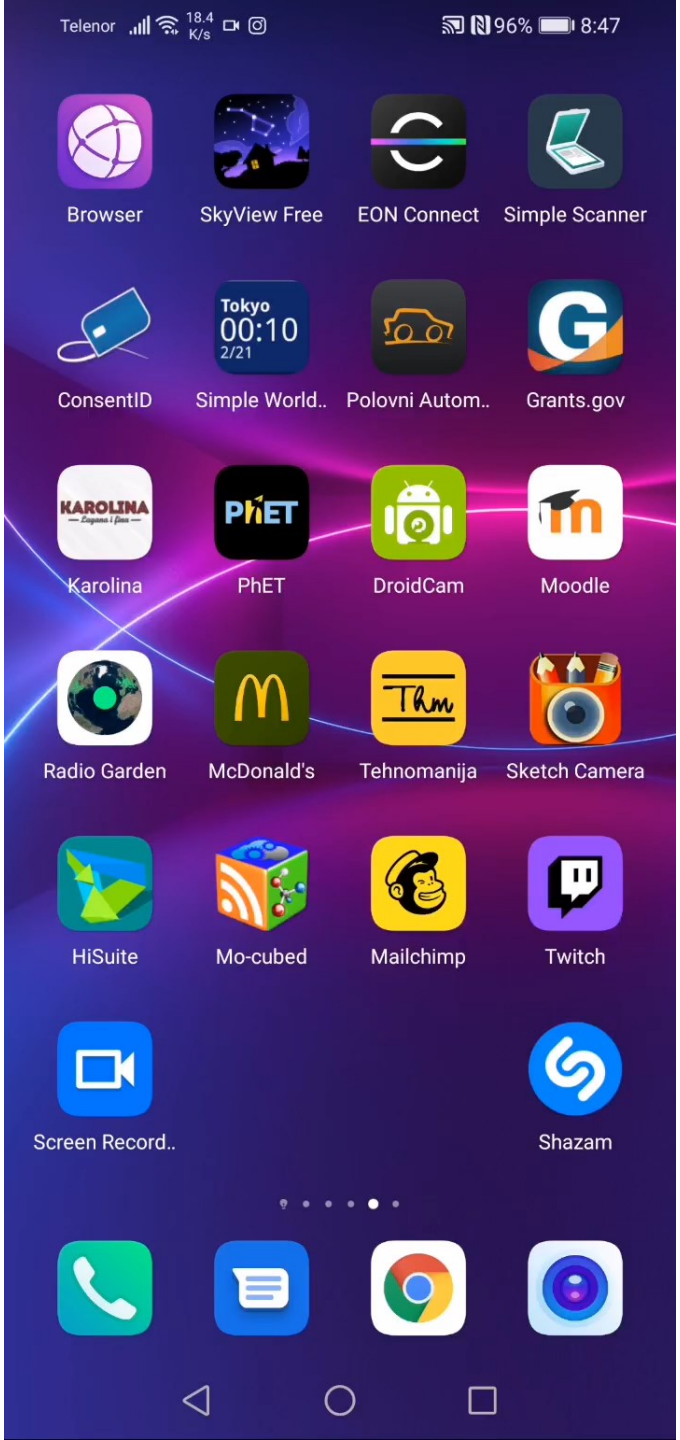
Received: 9 March 2012 / Accepted: 2 May 2012 / Published online: 29 May 2012

Abstract The aim of this study is to investigate the active components of representative drugs for blood pressure regulation by applying quantum mechanical computer codes and comparison of the same for the sake of obtaining knowledge about the properties associated with the electronic structure of given molecules. The study included three well-known, but not theoretically investigated enough, active components of β-blockers: acebutolol, metoprolol and atenolol. The results are in agreement with the experimental data and were used for initial assumptions concerning the degradation of these compounds.

Keywords Aromaticity · β-blockers · NBO · NMR parameters · NPA · Stability

treatment plant (STP) and of the refractoriness with respect to abiotic and biotic (natural) transformations. Although the concentrations at which they are normally found in the aquatic environment are in the range of micrograms per liter to nanograms per liter [1, 2], no indications exist for the most part of them that allow to rule out possible interactions with living organisms. Hundreds of tons of pharmaceuticals are annually prescribed in Europe and consequently discharged modified or as metabolites in sewage effluents [3].

Amongst the considerable number of pharmaceuticals that can be detected in receiving effluents, β-blockers are characterized by increasing use in recent years, and, as a consequence, an increasing presence in aqueous effluents is envisaged. They belong to the group of cardiovascular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18.4 K/s
96%
8:47
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SkyView Free
EON Connect
Simple Scanner
ConsentID
Tokyo
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2/21
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Polovni Autom..
Grants.gov
KAROLINA
Karolina
PhET
PhET
DroidCam
Moodle
Radio Garden
McDonald's
Tehnomanija
Sketch Camera
HiSuite
Mo-cubed
Mailchimp
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Screen Record..
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