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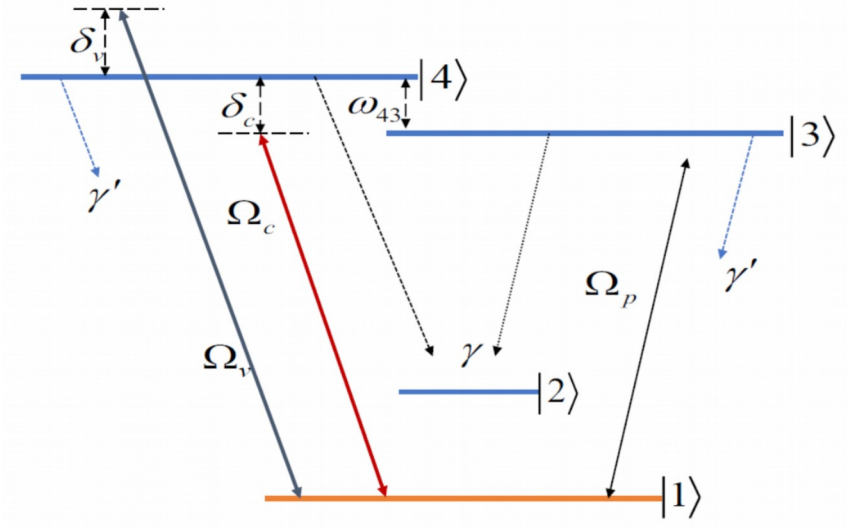
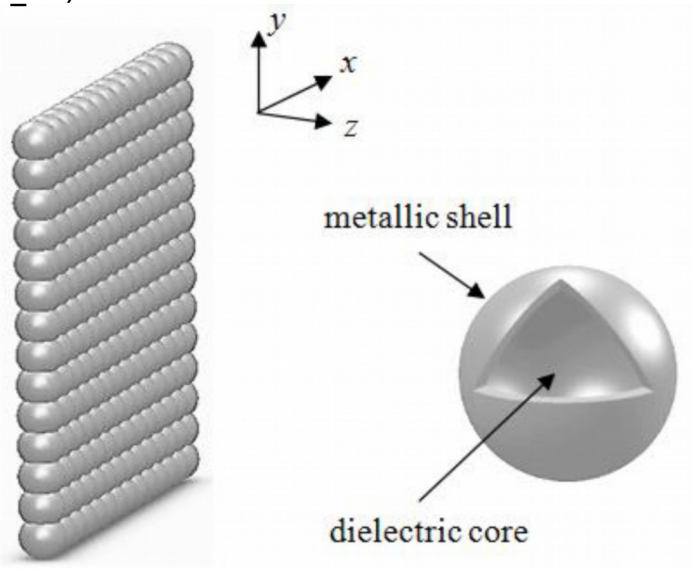
ATOMFIZIKAS UN SPEKTROSKOPIJAS INSTITŪTS

Project 1:
Electromagnetically Induced Grating near Plasmonic Nanostructure

This work was supported by the **trilateral Grant No. LV-LT-TW/2023/10 "Coherent Optical Control of Atomic Systems" by the Ministry of Education and Science of the Republic of Latvia, the Research Council of Lithuania, and the National Science Council of Taiwan** (project leader Prof. Marcis Auzinsh, LU_LC)





(a) Double V -type atomic system interacting with a coupling light with Rabi frequency Ωc, a vortex beam with Rabi frequency Ωv and a probe light with Rabi frequency Ωp;

(b) PN arranged in a 2D array at a distance d from the 4-level quantum system.

- The two coherent coupling fields are given by:

$$\Omega_c = \Omega[\sin(\pi x/\Lambda_x) + \sin(\pi y/\Lambda_y)],$$
$$\Omega_v = \Omega e^{-r^2/w^2}(r/w)^{|l|}e^{il\phi}.$$

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Project 1: Electromagnetically Induced Grating near PN

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H_{int}, \rho] + \mathscr{L}\rho,$$

-density matrix equations of motion, last term describes the effects of different decay mechanisms

$$\chi = \gamma_{31}\rho_{12}$$

-optical susceptibility of the medium

$$T(x,y) = e^{-Im(\chi)L} e^{iRe(\chi)L},$$

-transmission function for interaction length L, first/second term corresponds to amplitude/phase modulation

$$E(\theta_x,\theta_y) = \int_0^1 T(x,y)\exp(-i2\pi x\sin\theta_x)\exp(-i2\pi y\sin\theta_y)dxdy$$

-Fraunhofer diffraction of single space period

$$I_p(\theta_x,\theta_y) = |E(\theta_x,\theta_y)|^2 \frac{\sin^2(M\pi R_x sin\theta_x)}{M^2\sin^2(\pi R_x\sin\theta_x)} \frac{\sin^2(N\pi R_y\sin\theta_y)}{N^2\sin^2(\pi R_y\sin\theta_y)}$$

-Fraunhofer (far field) diffraction

$\Theta x,y$-diffraction angles

$Sin\Theta x=m/x$; $sin\Theta y=n/y$-diffraction orders

$Rx,y=\Lambda x,y/\Lambda$

M,N-number of spatial periods in the grating

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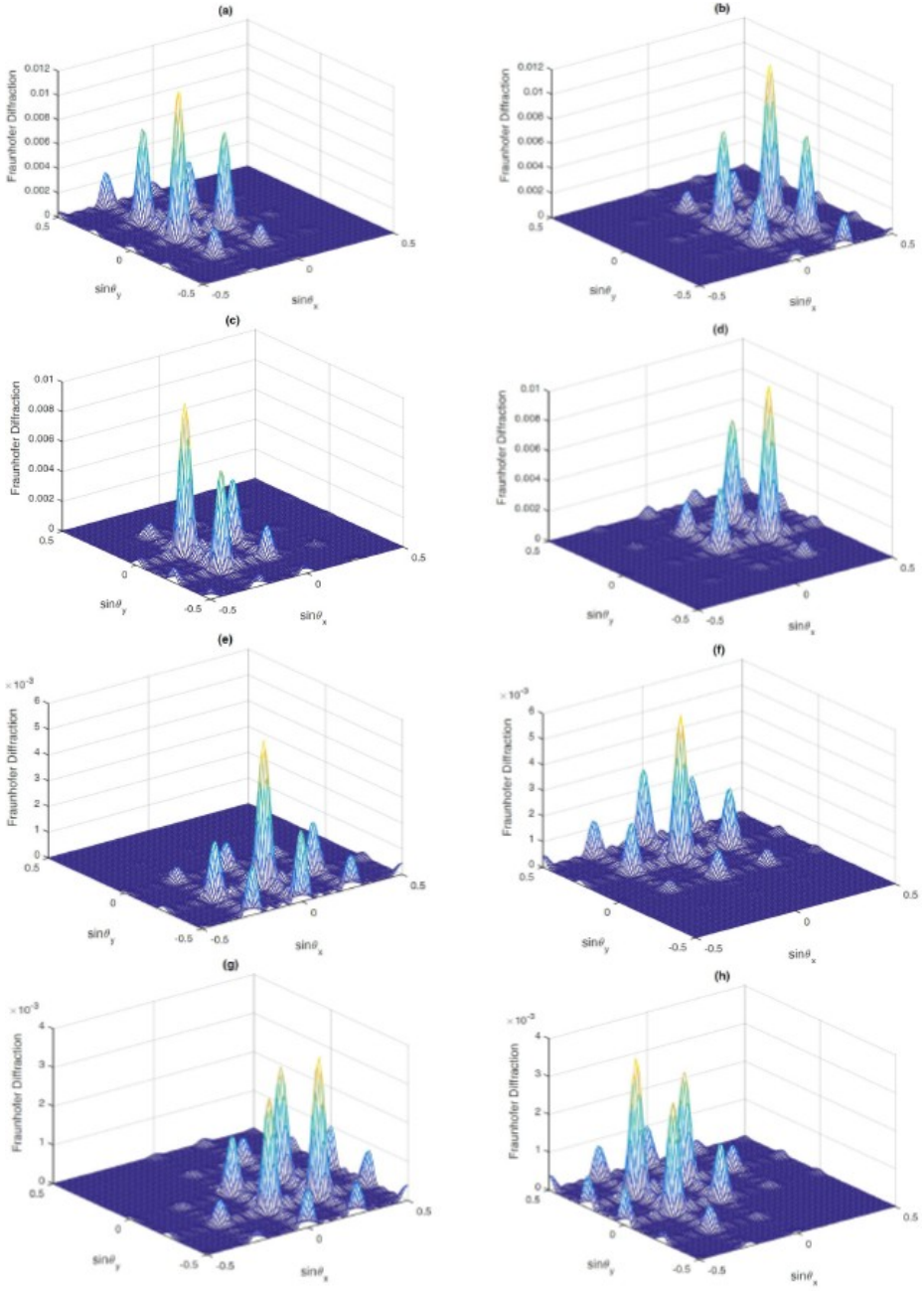

Distance d (in nm)	$\Gamma_\perp$ (in units Γ_0)	$\Gamma_\parallel$ (in units Γ_0)
2.2	35.668	0.086
6.6	8.080	0.015
19.8	0.277	0.0008965
22	0.183	0.0044

Fraunhofer diffraction pattern as function of sin θx and sin θy at distance d= 2.2nm

(a) l = 1; (b) l = −1; (c) l = 2; (d) l = −2;
(e) l = 3; (f) l = −3; (g) l = 4; (h) l = −4.

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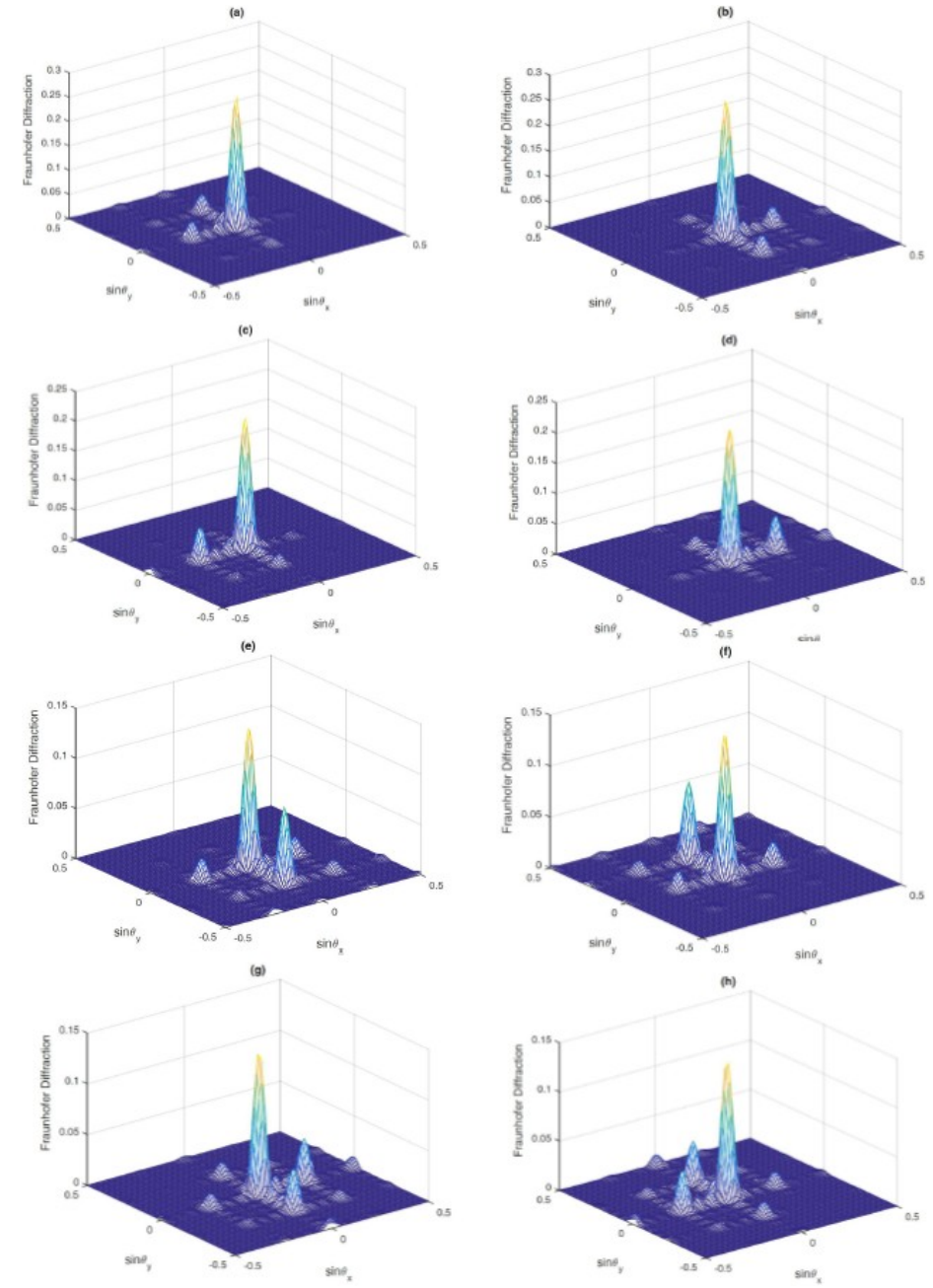

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- **This work is published in:**

S. H. Asadpour, T. Kirova, H. R. Hamedi, V. Yannopapas, and E. Paspalakis, European Physical Journal Plus 138, 246 (2023)

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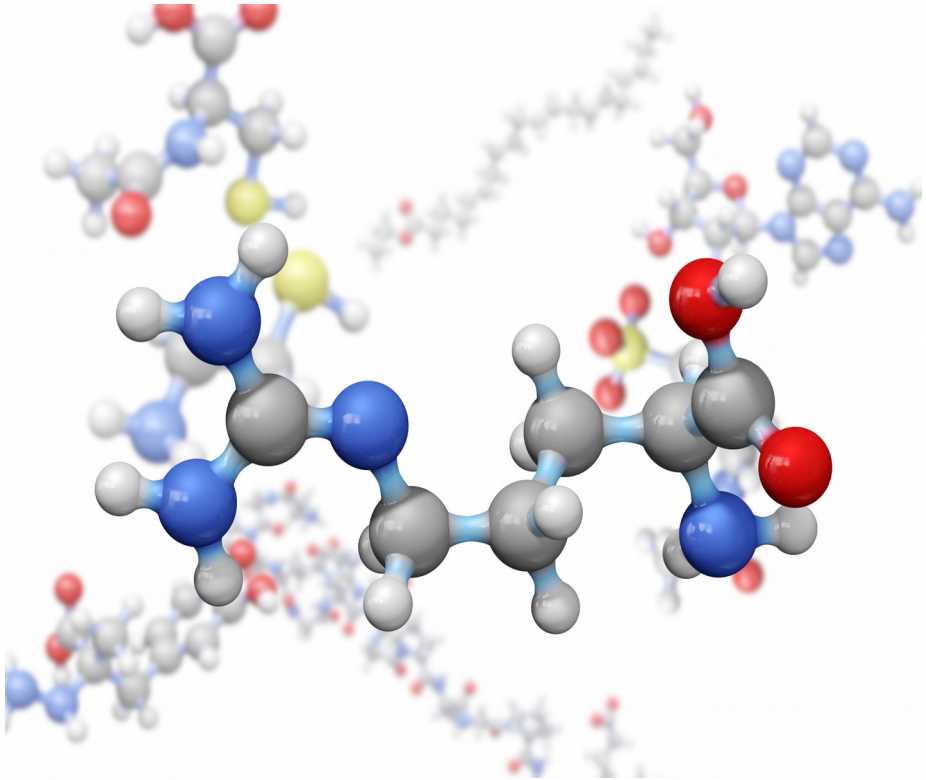
Project 2:
Numerical studiesof the impact of radiation on amino acids (valine, tyrosine)

This work was supported by **COST action CA18212 "Molecular Dynamics in Gas Phase" (MD-GAS) (2019-2024)**



https://www.shimadzu.se/amino-acids-analysis

Amino acids are the structural units of the proteins. By joining together, amino acids form peptides (short polymer chains) or polypeptides / proteins (longer polymer chains). Non-protein amino acids also have important roles as metabolic intermediates, such as in biosynthesis, or are used to synthesize other molecules.
For example, tryptophan is a precursor of the neurotransmitter serotonin, serine plays a crucial role in the metabolism and signaling activities in living organisms, while threonine is an important constituent of collagen, elastin, and enamel protein.

COST Action CA18212
MD-GAS
Molecular Dynamics in the GAS phase

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Project 2:
Numerical studies of the impact of radiation on amino acids (valine, tyrosine)

- Radiation field created by a single moving charge: the electric field, along with the corresponding magnetic field, constitute the radiation field of a moving charge:

$$\mathbf{E}(\mathbf{r},t) = \frac{q}{4\pi\epsilon_0}\left\{\frac{\hat{\mathbf{R}}}{(1-\hat{\mathbf{R}}\cdot\beta)^3 R}\times\frac{1}{c}\left[(\hat{\mathbf{R}}-\beta)\times\dot{\beta}\right]\right\} \quad ; \quad \mathbf{B}(\mathbf{r},t) = \frac{1}{c}\hat{\mathbf{R}}\times\mathbf{E}(\mathbf{r},t)$$

The effects of the E field are larger by a factor of $1/\alpha$ ($\alpha=1/137$ is the fine structure constant) .Therefore as first approximation we will neglect the terms of the oscillating B field in the Hamiltonian and leave only the ones including the E field.

- The effects of the B field of the EM radiation will be only accounted for by using the method of Anisotropic Gaussian type orbitals (AGTO). In cylindrical coordinates the j th AGTO has the form, resulting in elongation of the electron densities along the B field direction:

$$\chi_j(\rho,z,\phi) = N_j \rho^{n_{\rho_j}} z^{n_{z_j}} e^{-\alpha_j\rho^2-\beta_j z^2} e^{im_j\phi}, j=1,2,3\ldots,$$

, where n, l, m describe different molecular quantum numbers.

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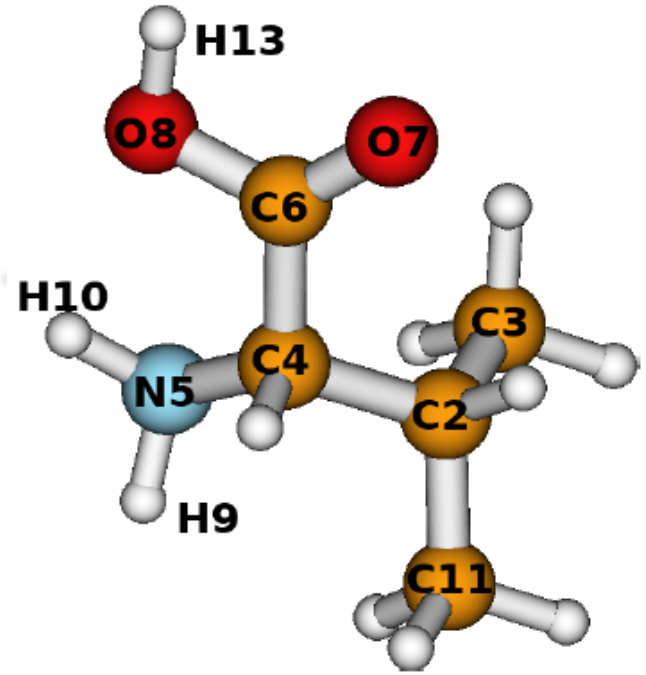
Project 2:
Numerical studies of the impact of radiation on amino acids (valine)



The view of one of the most stable valine conformers

Valine is an α-amino acid which is used in protein biosynthesis and thus is essential in humans and must be obtained through the diet. In sickle-cell disease it substitutes for the hydrophilic glutamic acid, and since valine is hydrophobic, the hemoglobin is prone to abnormal aggregation

The measured mass spectra of the valine molecule upon interaction with a high-energy electron beam have been studied (*J. Tamuliene et.al, Horizons in World Physics. Volume 305, Nova Science Publishers, 2021*.)

The most important results obtained in that study are as follows:

-the intensities of the peaks with respect to that of the m/z = 72 fragment (corresponding to C4H10N+) significantly changed.

-the peak intensity of the m/z = 27−29 fragments (CH2N, CH3N) decreases differently with increasing the irradiation dose;

-the intensity of the m/z = 45 (CHO2+) fragment increases because the CO2 molecule joins the H atoms formed due to irradiation, whereas the m/z = 55 and 56 (C4H7, C3H5N and C4H9, C2H2NO) fragments result from the decomposition of not only the parent valine molecule but also the C4H9N or C2H3NO2 fragments formed under irradiation

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Project 2:
Numerical studies of the impact of radiation on amino acids (valine)

E field, a.u.	Valine in E field	Valine in EM field (s, p orbitals)	Valine in EM field (p orbitals)
0.3	stable	stable	stable
0.4	unstable*	unstable*	unstable*
0.5	unstable*	unstable*	CO_2, CH_3, H, C_3H_7N
0.6	$CO_2, 2H, C_4H_9N$, $CO_2, 3H, C_4H_8N$	$CO_2, 3H, C_4H_8N$	CHO_2, CH_2, H, C_3H_7N
0.7		C, 2O, 2H, C_4H_9N	$CO_2, CH_2, 2H, C_3H_7N$

Effects of the magnetic field became more important with the increase of the electric dipole field strength.
-the decomposition of valine occurs at a lower strength of the dipole electric field.
-the fragments formed with and without the inclusion of the magnetic field effects are different.

Formation of the CHO2 fragment occurs only when the magnetic field effects are included to the basis set of the p− orbitals. This effect is not seen when only the influence of the electric field is taken into account.

According to the experimental studies the intensity of the m/z = 45 (CHO2+) fragment increases in the mass spectra of the valine, which is explained as the CO2 fragment bonding to the H atoms formed due to the irradiation. Better fitting of the experimentally obtained spectra.

- **This work is published in:**

  T. Kirova and J. Tamuliene, Materials 16(5), 1814 (2023)

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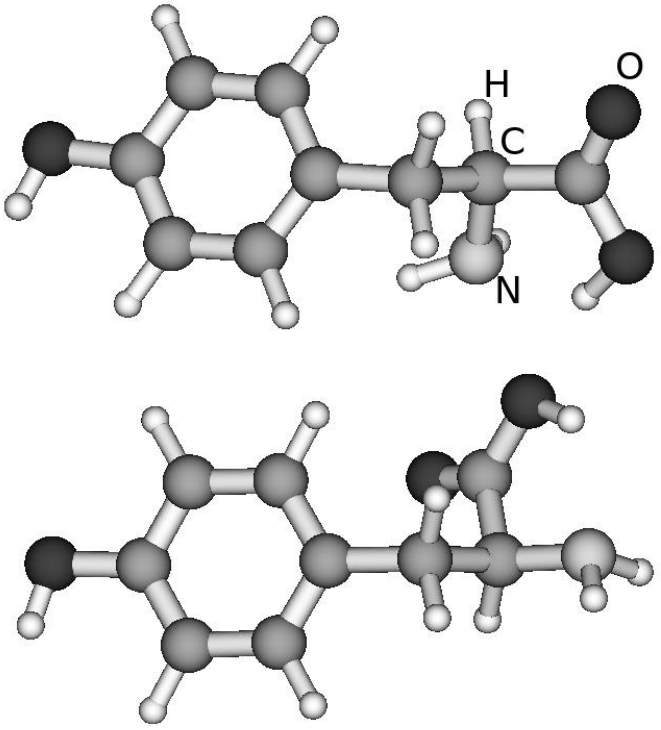
Project 2:
Numerical studies of the impact of radiation on amino acids (tyrosine)



The view of the most stable conformer of tyrosine obtained without (on the top) and with (on the bottom) the inclusion of the dipole electric field

Tyrosine is a nonessential amino acid the body makes from another amino acid called phenylalanine. It is an essential component for the production of several important brain chemicals called neurotransmitters, including epinephrine, norepinephrine, and dopamine.

Experimental Details:

-The experimental apparatus is typical crossed-beam setup based on a M I1201 magnetic mass spectrometer

-The tyrosine molecular beam having a ~ 1010 molecule/cm3 density was produced by an effusion source operating within the temperature range not exceeding 150◦C, thus, excluding possible thermal degradation of the molecule

-The overall time interval between molecule irradiation and measuring the mass spectra exceeded at least 300 hours, allowing any reversible changes in the molecular structure to relax, with no final effect on the mass spectra measured

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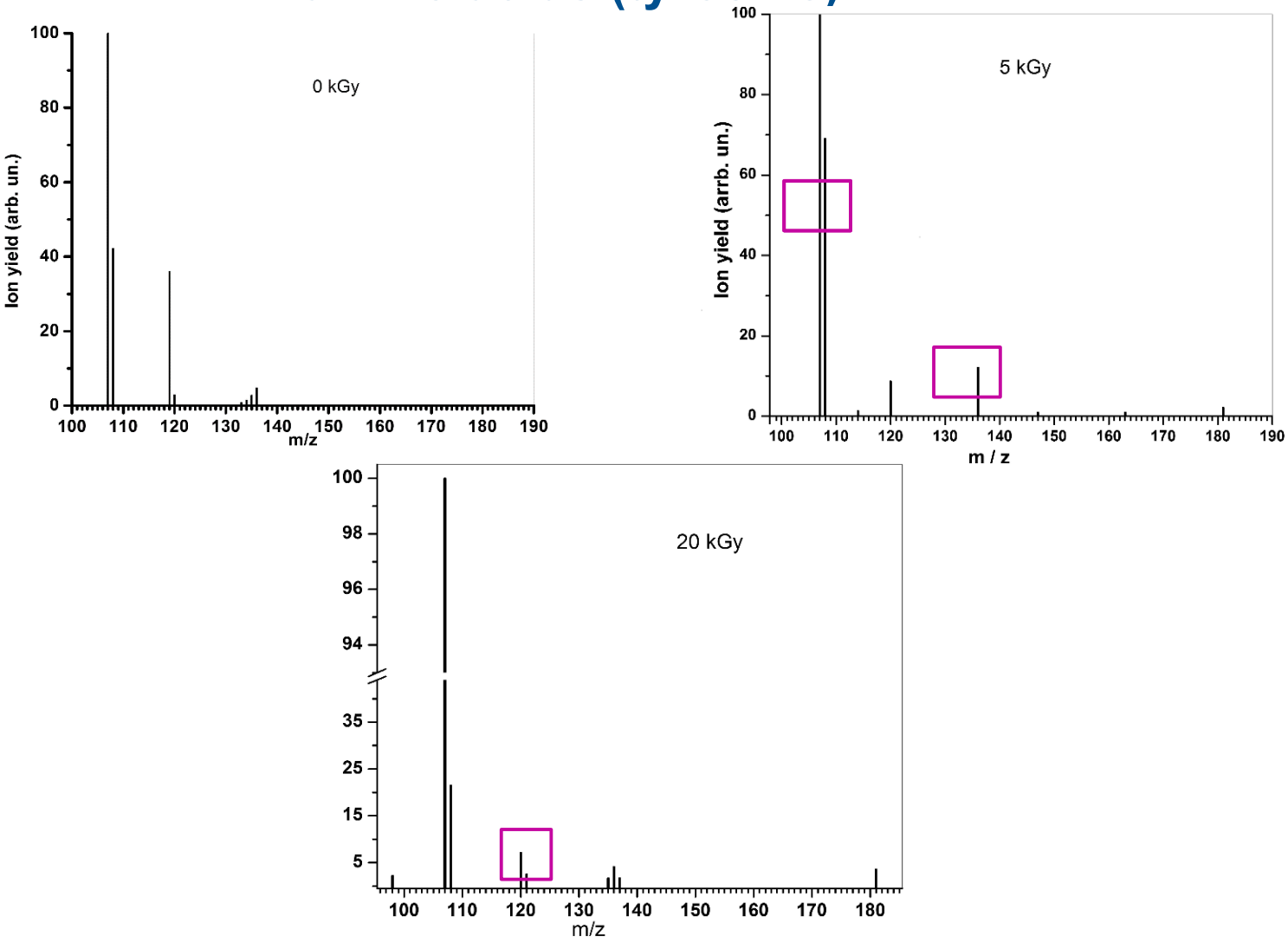

Comparison of the mass spectra of non-irradiated and electron-irradiated (at the 5kGy and 20kGy doses) tyrosine molecules measured at the 70eV incident electron energy in the mass range 100- 190 a.m.u.

The intensity of the m/z = 108 and 136 fragments increases at 5kGy and decreases at 20kGy.

The peak representing the m/z = 119 fragment at 0kGy disappeared, and a lower peak at m/z = 120 occurs at 5kGy and 20kGy

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Project 2:
Numerical studies of the impact of radiation on amino acids (tyrosine)

-We observe significant differences in the geometrical structure of tyrosine with and without the inclusion of an electric field- the rotation and bending of COOH- CH-NH2 with respect to the phenol ring is seen.

-The decomposition of the molecule to COOH, H, and C8H9NO is revealed in the 0.31a.u. and larger dipole electric field. The splitting to COOH and C8H9N O is also predicted or dipole electric field with strength equal to 0.7a.u.

-The obtained results indicate slightly different consequences of tyrosine splitting in the electromagnetic field, i.e. CO2,C8H9NO, and two H atoms could be formed. These results give a better match with the experimental spectra.

-The increase of the m/z=108 peak (corresponds to C7H8O) at 5kGy indicates the facilitation of the intramolecular hydrogen migration process, where C7H7O binds with the H atom.
-The m/z = 136 fragment (corresponds to C8H10NO) is formed due to a loss of CHO2 due to the irradiation, leading to increase in the peak intensity at 5kGy.

-The m/z = 119 and 120 fragments (correspond to C8H7O and C8H8O, respectively) are formed when tyrosine lost COOH, N H2, and, in the case of m/z = 119, a proton, as a consequence of the C-C bond break. The m/z = 120 peak is formed at various irradiation doses because the C-H bond break is quenched and, as a consequence, this peak appeared instead of the m/z = 119 one.

- This work is published in:

J. Tamuliene, T. Kirova, L. Romanova, V. Vukstich, A. Snegursky,
European Physical Journal D, 77 13 (2023), topical issue
on "Physics of Ionized Gases and Spectroscopy of Isolated
Complex Systems: Fundamentals and Applications

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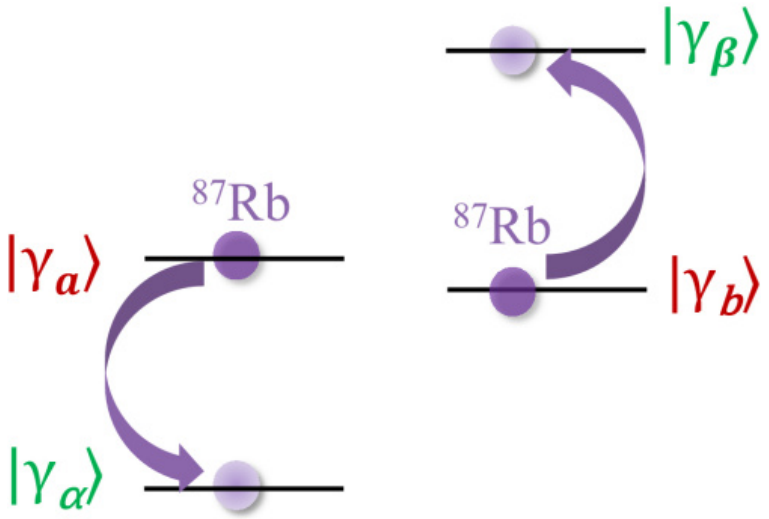
Project 3:
Rydberg-Rydberg Interaction Strength and Dipole Blockade Radii in the Presence of Förster Resonances

This work was supported by the **trilateral Grant No. LV-LT-TW/2023/10 "Coherent Optical Control of Atomic Systems" by the Ministry of Education and Science of the Republic of Latvia, the Research Council of Lithuania, and the National Science Council of Taiwan** (project leader Prof. Marcis Auzinsh, LU_LC)



Schematics of a Förster resonance transition with initial states |γa⟩, |γb⟩ and final states |γα⟩, |γβ⟩.

-Achieving substantial blockade radius is crucial for developing scalable and efficient quantum communication and computation.

- In our theoretical study we presented the enhancement of the Rydberg blockade radius by utilizing Förster resonances (FR).

FR occur when the energy difference between two initial Rydberg states closely matches the energy difference between the corresponding final Rydberg states, giving rise to a resonant energy transfer process.

-We numerically calculate the ^{87}Rb–^{87}Rb Rydberg atomic pair, enabling us to accurately estimate the van der Waals interaction.

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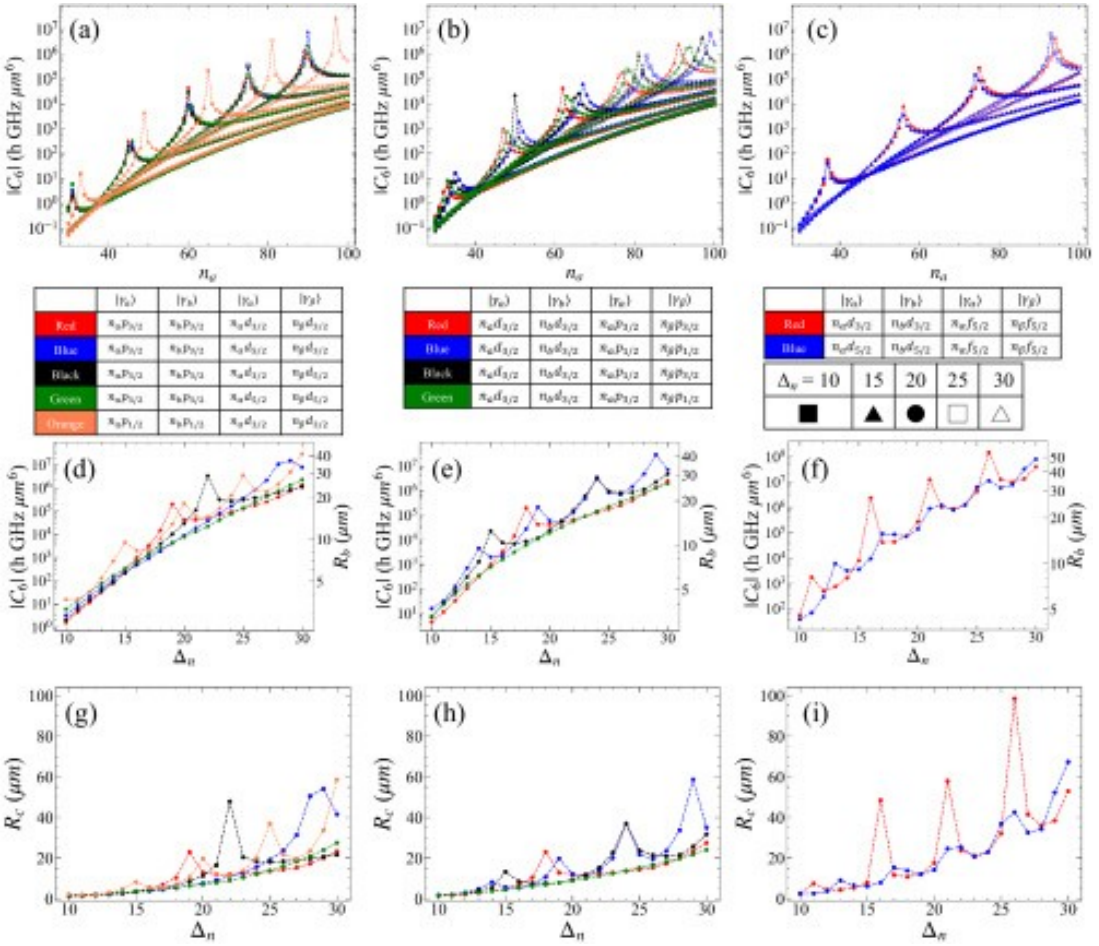

The van der Waals coefficient C_6 versus principal quantum number n_a (a-c); the van der Waals coefficient C_6 versus the Förster defect Δ_n (d-f); dipole blockade radii R_c versus the Förster defect Δ_n (g-i).

-Our investigations showed that when the principal quantum numbers of two Rydberg states differ only slightly, the Förster transition is not able to achieve large blockade radius.

-However, when the principal quantum numbers differ significantly, we can substantially improve the Rydberg blockade radius,

-For example the largest blockade radius in all possible channels is 53 μm for the transition of $98d3/2+124d3/2 \rightarrow 97f5/2+122f5/2$ (red one for Δn=26) with the Förster defect of 0.16 MHz and $C_6 = -1.4\times10^8$ GHz μm^6.

-This is also the largest radius reported in the literature so far.
These outcomes are opening up exciting possibilities for advancements in quantum information processing and quantum communication technologies.

This work is published in:

C. E. Wu, T. Kirova, M. Auzins, and Y.-H. Chen, Optics Express 31(22), 37094 (2023)

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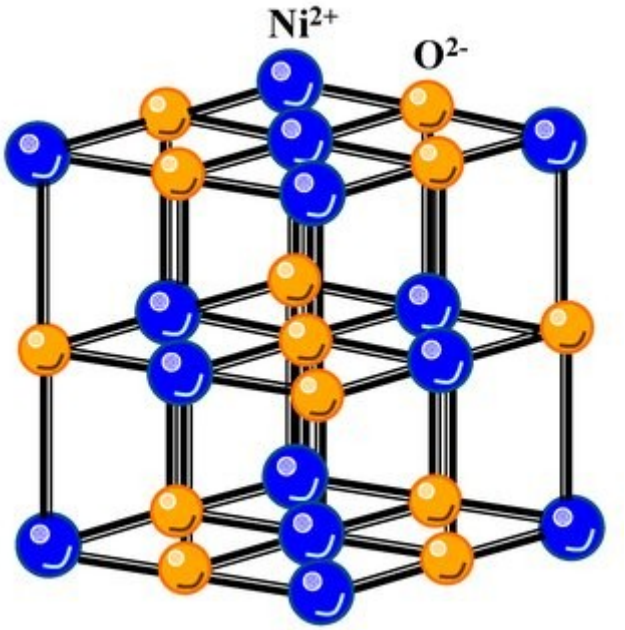
Project 4: Structural, electronic and optical properties of NiO from first principles

Supported by the Z-LZP103-ZF-N-109 project "Jaunas kodola apvalka nano šķiedras, kas veidotas, izmantojot koaksiālu elektrisko vērpšanu fotokatalītiskiem lietojumiem" (project leader Dr. Roman Viter) and in collaboration with Dr. Andris Gulans from LU_FMOF



Nanomaterials 2020, 10(4), 636

NiO crystallizes in a rock-salt crystal structure with a=b=c=2.899Å, V=17.225Å^{-3}

Due to a strong electron correlation in 3d orbitals, it has an optical bandgap of 3.4–4.0 eV

At the nanoscale NiO is a p-type semiconductor, which might be important for multiple technological applications:

-catalysis,
-batteries, solar cells;
-functional sensor layers in chemical sensors,
-optoelectronic, photovoltaic materials,
-displays,
-lighting diodes, lasers, etc.

The magnetic behavior in bulk samples of nickel oxide was seen as an antiferromagnetic ordered system. This characteristic is different as it occurs at the nanoscale (ferromagneism, Mott-insulator, spin-surface magnetism).

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Project 4: Structural, electronic and optical properties of NiO from first principles

The Journal of Chemical Physics ARTICLE scitation.org/journal/jcp

CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficier and accurate electronic structure calculations

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[7] Centre of Policy Studies, Victoria University, Melbourne, Australia

-CP2K is a quantum chemistry and solid state physics software package that can perform atomistic simulations of solid state, liquid, molecular,periodic, material, crystal, and biological systems.

-CP2K provides a general framework for different modeling methods such as DFT using the mixed Gaussian and plane waves approaches.

-CP2K can do simulations of molecular dynamics, Monte Carlo, vibrational analysis, core level spectroscopy, energy minimization.

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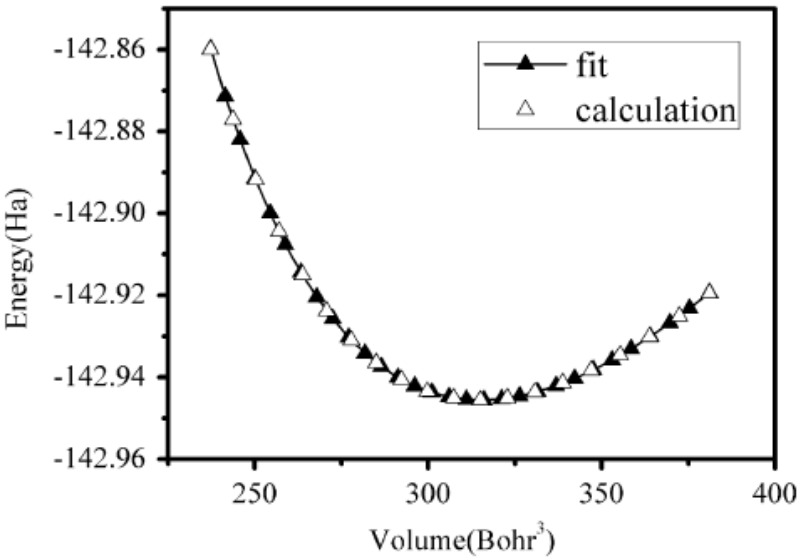
Project 4: Structural, electronic and optical properties of NiO from first principles

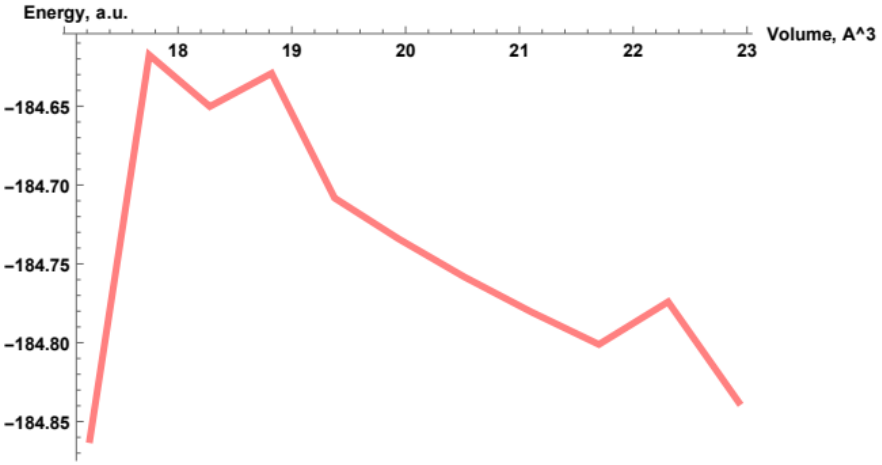
-We are currently performing calculations of the total energy as a function of the unit-cell volume within 10% around the equilibrium cell volume.

-Calculated energies will be fitted to a third-order empirical function from which we can obtain various structural properties, such as the ground state energy E_0, the equilibrium volume V_0, the bulk modulus B_0, the pressure derivative of bulk modulus B_0'.

-We will compare the calculated structure parameters with previous experimental and theoretical studies, after which we will proceed to determine the band structure, density of states, linear and nonlinear optical susceptibilities of NiO.



F. Kong at al. Physica B 404 (2009) 2340–2344



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Educational Workshops

1.“Our Beautiful Minds: An Introduction to Neurodiversity at Work”, webinar, 5.12.2023, organized by “SNAC: supporting neurodiversity at CERN

2. GENERA General Assembly 2023, 24-25 October 2023, hybrid workshop, organized by GENERA network

3. 1st Training School of the COST action CA21101 COSY "Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications”, 19-22 September, Belgrade, Serbia

4. GENERA workshops in Physics module II: Skills needed to build a (successful) career, 20 April 2023, virtual workshop, organized by GENERA network

5.UniSAFE webinar on ”Setting up and Implementing Institutional Policies to Combat Gender-Based-Violence in Academia-The 7P Framework”, 18, 25 April, and 2 May 2023, organized by UniSAFE project “Ending gender-based violence’

6. UniSAFE webinar on “Create Successful Awareness-raising Campaigns on Gender-Based Violence at Your University”, 28 march 2023, organized by UniSAFE project “Ending gender-based violence’

Www.conference2go.com
/education/

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Plan for 2024

1. Continue collaborations within the COST Action 18212 "Molecular Dynamics in the GAS-phase" (MD-GAS),(2019-2024), *country representative*

2. Continue collaborations within the COST action CA18222 "Attosecond Chemistry" (AttoChem), (2019-2024), *country representative*

3. Start new collaborations within the COST action CA21101 (2022-2026) "Confined Molecular Systems: from a New Generation of Materials to the Stars" (COSY), *Latvia country representative*

4. Start new collaborations within the COST action "Topological textures in condensed matter" (Polytopo), (2023-2026), *country representative, waiting for funding results??*

5. Continue work on GENERA:"Gender Equality Network in the European Research Area", *country representative*

6. Continue work on Trilateral grant of the Latvian, Lithuanian, and Taiwanese Research Councils "*Coherent Optical Control of Atomic Systems*" (project leader Prof. Marcis Auzinsh), *project coordinator and co-PI* (2022-2024)

7. Continue work on LZP project "Jaunas kodola apvalka nano šķiedras kas veidotas izmantojot koaksiālu elektrisko vērpšanu fotokatalīstiskiem letojumiem" (leader Dr. Roman Viter) (2022-2024)

8. Coordinate the Horizon Europe MSCA-SE project *"Q-DYNAMO: Quantum Dynamic Control of Atomic, Molecular and Optical Process"*, *project coordinator* (2024-2027)

9. Submit/ Resubmit "Horizon Europe" (IF, TWINNING), "LZP", "Latvia Lithuania, and Taiwan", "Postdoc Latvia" project applications

10. Publications, conferences and scientific visits
11. Looking for MS, PhD and postdocs

Teodora Kirova, LU_ASI