Summary of main results and scientific contributions

of Assistant Professor Tina Radmilova Tasheva, PhD,
presented for participation in a competition for "Associate Professor" position
in scientific specialty 5.6. Materials and Materials Science (Silicate Materials),
announced by UCTM in the State Gazette, issue 64/05.08.2025

The candidate is participating in the competition with 20 publications: 10 listed in the habilitation reference (Group B indicators) and 10 outside the habilitation reference (Group G indicators). All 20 publications are in journals indexed in the Scopus and/or Web of Science databases. The citations observed for the publications participating in the competition total 145, all of which are indexed in Scopus. The candidate's Hirsch index (h-index) is 8, based on all publications. The scientific work of the candidate has been presented at 63 international, national, and university scientific conferences, including 51 poster presentations and 12 oral reports. Senior Assistant Professor Tina Tasheva has served as: Principal investigator of 5 projects funded by the Research and Development Sector (RDS) at UCTM, Member of research teams in 6 RDS projects at UCTM, Principal investigator of 3 national and 1 international project funded by the Bulgarian National Science Fund (NSF), Member of research teams in 4 national and 1 international NSF projects, Member of a research team in a project under the National Recovery and Resilience Plan of the Republic of Bulgaria, Supervisor of 8 diploma theses.

The total number of points required for holding the academic position of Associate Professor, according to the minimum national and additional institutional requirements (UCTM), is 500 points. The candidate applies with a total of 734.9 points.

The scientific interests and research activities of the candidate are in the field of materials science, particularly in the glass science, nonlinear optics, bioactive glasses for medical applications, and structural characterization of materials.

The scientific contributions are summarised in four main areas:

1. Synthesis of oxide glasses and investigation of the influence of their structure on optical and dielectric properties. Application of the polarizability approach to oxide glasses.
    - 1.1. Vanadate glasses in the MeOn-BaO-V_2O_5 (where Me = Ti, Zn, Te) systems (publications 1, 2, 3, 5 from indicator Г7);
    - 1.2. Bismuthate and borate glasses in the Na_2O-Bi_2O_3-B_2O_3 system (publication 4 from indicator Г7);
    - 1.3. Tellurite glasses in the systems V_2O_5-BaO-TeO_2 (publication 6 from G7) and TeO_2-V_2O_5-MoO_3 (publication 7 from Г7);
    - 1.4. Glasses in the systems Na_2O–CaO–SiO_2–Fe_2O_3, (Na_2O–CaO–SiO_2)/Fe_2O_3, and Na_2O–BaO–ZrO_2–TiO_2–SiO_2–B_2O_3–Al_2O_3 (publications 6, 7, and 8 from indicator B4).

2. Synthesis and characterization of bioactive glasses and glass-ceramics.
    - 2.1. Bioactive borate glasses (publications 9 and 10 from indicator Г7);
    - 2.2. Bioactive silicate and borosilicate glasses and glass-ceramics (publications 9 and 10 from indicator В4).
3. Electronic polarizability and group optical basicity (publications 1, 2, 3, 4, and 5 from indicator В4).
4. Characterization of carbonation products from cement kiln dust (publication 8 from indicator Г7).

1. Synthesis of oxide glasses and study of the influence of their structure on optical and dielectric properties

The first group of papers presented by the candidate belongs to group "Г" and is related to the synthesis and characterization of oxide glasses from the systems MeO_n-BaO-V_2O_5 (Me = Ti, Zn, Te), Na_2O-Bi_2O_3-B_2O_3, V_2O_5-BaO-TeO_2, and TeO_2-V_2O_5-MoO_3. This research topic was developed in the Department of Silicate Technology at the University of Chemical Technology and Metallurgy (UCTM).

The candidate's main activities were focused on the synthesis, structural characterization, and determination of the thermal parameters of the materials. The polarizability approach was applied to this group of glasses, and their electronic polarizability and optical basicities were determined. The relationship between the structure and the optical characteristics of the glasses was investigated. The measurement of the dielectric properties of glasses from the TeO_2-BaO-V_2O_5 system was carried out in collaboration with the Department of Physics at UCTM. The studies on the TeO_2-V_2O_5-MoO_3 system resulted from a project funded by the National Science Fund, coordinator: assistant Professor Tina Tasheva, which was completed and highly evaluated.

Another group of papers presented by the candidate in this section belongs to group "В" and focuses on glasses from the systems Na_2O-CaO-SiO_2-Fe_2O_3 and Na_2O-BaO-ZrO_2-TiO_2-B_2O_3-SiO_2-Al_2O_3. This research was carried out in the Department of Physics at UCTM, and the studies were part of a project funded by the National Science Fund, in which the candidate participated as a member of the research team. In this group of publications, the candidate contributed to the determination of certain physicochemical parameters, the prediction of the refractive index of the glasses, and structural characterization using infrared spectroscopy.

1.1. Vanadate glasses in the systems MeO_x–BaO–V_2O_5, where Me = Ti, Zn, Te (publications 1, 2, 3, 5 from indicator Г7).

Glasses in the systems TiO_2-BaO-V_2O_5, ZnO-BaO-V_2O_5, and TeO_2-BaO-V_2O_5 were synthesized using the melt-quenching technique. X-ray diffraction (XRD) analysis confirmed the amorphous nature of all samples. The ternary glasses exhibit low glass transition temperature

(Tg) and crystallization temperatures (Tx), with similar values across all systems, although TeO_2-based glasses showed slightly higher Tg and Tx with increasing TeO_2 content.

The density of the glasses decreases with increasing content of the corresponding oxide, indicating that replacing BaO with TiO_2, ZnO, or TeO_2 leads to expansion of the glass network and reduction in density. Differences were also observed in the refractive index and oxide ion polarizability. All glasses possess high refractive indices (2.112–2.421), with ZnO-based glasses showing the highest values (up to 2.421), while TeO_2-based glasses exhibited a narrower range (2.16–2.19). The oxide ion polarizability was relatively high for all systems (2.65–2.725 $Å^3$), explaining their strong linear optical properties. The optical basicity values were also high and similar across the three systems (1.040–1.057), suggesting the presence of highly polarizable chemical bonds.

The third-order nonlinear optical susceptibility, $\chi_{(3)}$, calculated using Miller's rule, also showed significant variation among the systems: TiO_2-based glasses had χ(3) in the range 0.76–1.1×10^{-12} esu, ZnO-based ones ranged from 0.58-2.24×10^{-12} esu, while TeO_2-based glasses showed 0.72 - 0.85×10^{-12} esu. The highest $\chi^{(3)}$ values were observed in ZnO-based glasses, indicating their potential for nonlinear optical applications.

The average single bond strength ($B_{M\text{–}O}$) and the interionic interaction parameter (A) indicated relatively weak chemical bonds, with $B_{M\text{–}O}$ ranging from 251 to 295 kJ/mol and A from 0.049 to 0.055 $Å^{-3}$. Infrared (IR) spectra confirmed the presence of Ba...O=V, V–NBO (non-bridging oxygens), V–O–Ti, V–O–Zn, V–O–Te, and V–O–V bonds. Structural models were proposed, suggesting the presence of VO_5, VO_4, TiO_4, ZnO_4, and TeO_3 groups in the glasses. The high polarizability of oxide ions in these bonds is the key factor behind the observed linear and nonlinear optical properties, including the high refractive indices and nonlinear refractive behavior.

The dielectric properties of glasses from the TeO_2-BaO-V_2O_5 system were investigated by measuring dielectric permittivity, dielectric loss, and frequency-dependent conductivity in the range of 100 Hz - 1 MHz at room temperature. Small polaron hopping between $V^{4+} \rightarrow V^{5+}$ in the vanadate chains was found to play a major role in these properties. The addition of TeO_2 caused three main structural changes that affected the dielectric parameters. For $TeO_2 < 10$ mol%, Ba^{2+} ions occupy interstitial positions in the glass network, where they can be located without disturbing the main structure, directly interacting with isolated V=O bonds (Ba^{2+}...O=V). Meanwhile, Te^{4+} ions become incorporated into the chains, indirectly affecting V=O bonds through O=V–O–Te linkages. Within the glass volume, the number of single distorted Te–O bonds increases, and for $TeO_2 > 10\%$, VO_4 units begin transforming into VO_5 structural groups. The replacement of BaO with TeO_2 leads to the formation of Te–O–V bonds, reducing dielectric losses, while the breaking of distorted Te–O bridges between VO_4 groups promotes transformation toward VO_5 units.

These findings demonstrate the possibility of controlling the dielectric properties through the substitution of BaO with TeO_2, opening opportunities for developing new functional amorphous materials in the TeO_2-BaO-V_2O_5 system with potential applications in advanced optical and electronic technologies.

1.2. Bismuthate and borate glasses in the system Na_2O–Bi_2O_3–B_2O_3 (publication 4 from indicator Г7).

Glasses in the Na_2O-Bi_2O_3-B_2O_3 system were synthesized using the conventional melt-quenching method. Several glass series with different compositions were prepared for the study: $(30–x)Na_2O·xBi_2O_3·70B_2O_3$ (x = 15, 20, 25 mol %), $(70–x)Na_2O·xBi_2O_3·30B_2O_3$ (x = 40, 50, 60 mol %), $(50–x)Na_2O·50Bi_2O_3·xB_2O_3$ (x = 45, 40, 35, 30 mol%), and $(40–x)Na_2O·60Bi_2O_3·xB_2O_3$ (x = 35, 30, 25 mol%). In addition, a glass with the composition $5Na_2O·70Bi_2O_3·25B_2O_3$ was also synthesized.

The oxide ion polarizability and optical basicity of the glasses were determined, showing broad variation ranges (1.545 - 2.457 $Å^3$ for polarizability and 0.589–0.990 for optical basicity). The glasses exhibited relatively high third-order nonlinear optical susceptibility, χ(3), in the range 0.90 - $2.42×10^{-13}$ esu, making them promising candidates for nonlinear optical applications.

The structure of the glasses was studied through the interionic interaction parameter, average single bond strength, and Fourier-transform infrared (FTIR) spectroscopy. It was found that glasses with a high Bi_2O_3 content show low interionic interaction values (0.224 - 0.051 $Å^{-3}$) and weak bond strength (377 - 198 kJ/mol), indicating the presence of weak chemical bonds within the glass network, as confirmed by FTIR spectra.

Analysis of the structural units revealed that glasses with low Bi_2O_3 content are primarily composed of pyroborate (B_4O_7) and orthoborate (BO_3) groups, while high Bi_2O_3 content leads to the presence of orthoborate BO_3 units linked with BiO_6 octahedra via mixed Bi–O–B bonds. These structural characteristics explain the observed optical and nonlinear properties and demonstrate the possibility of tuning χ(3) by adjusting the glass composition.

1.3. Tellurite glasses in the systems V_2O_5–BaO–TeO_2 (publication 6, G7) and TeO_2–V_2O_5–MoO_3 (publication 7, Г7)

Tellurite glasses in the systems V_2O_5-BaO-TeO_2 and TeO_2-V_2O_5-MoO_3 were synthesized using the melt-quenching technique.

In the TeO_2-BaO-V_2O_5 system, the glasses exhibit high oxide ion polarizability and optical basicity, indicating a strong electron-donating ability of the oxide ions. Structural studies revealed that substituting BaO with V_2O_5 leads to a more cross-linked glass network, composed mainly of ionic bonds of the Te–O–V, Te–O–Te, and V–O–V types, confirmed by FTIR spectroscopy. At low V_2O_5 content, the structure consists predominantly of distorted TeO_4 and isolated TeO_3 groups, while increasing V_2O_5 content results in the formation of VO_4 and VO_5 structural units, which organize into $(VO_4)_n$ zigzag chains connected by Te–O–V bridges. These structural transformations are responsible for the high refractive indices (n_0) and third-order nonlinear susceptibility χ(3), making these glasses suitable for nonlinear optical applications.

In the TeO_2-V_2O_5-MoO_3 system, four glass series were synthesized. It was found that V_2O_5 increases the free volume and the number of non-bridging oxygens (NBOs), while MoO_3 contributes to forming a more connected three-dimensional network. These glasses exhibit high oxide ion polarizability (2.560–2.657 $Å^3$) and optical basicity (1.018–1.042), again indicating strong electron-donating behavior. The refractive indices are high (2.100–2.281), whereas the interionic interaction parameters (0.048–0.055 $Å^{-3}$) and bond strengths (294–334 kJ/mol) are low, suggesting weak, predominantly ionic interactions.

FTIR spectroscopy confirmed the presence of Te–O–V, V–O–V, Mo–O–Mo, and Te–O–Te bonds linking different structural units within the glass network. The main structural groups include VO_5 trigonal bipyramids from $(VO_4)_n^{3n-}$ and $(V_2O_8)_n$ chains, MoO_5 bipyramids from $[Mo_2O_8]$ complexes, and distorted TeO_4 and TeO_3+1 bipyramids, associated with TeO_3 trigonal pyramids.

A shift of the V=O stretching vibration toward lower frequencies was observed in the presence of TeO_3+1 units, which possess high group optical basicity ($\lambda = 1.23$). This indicates weakening of the V=O bonds. The addition of V_2O_5 induces a transition from TeO_4 to TeO_3+1 and TeO_3 units, reflecting changes in the connectivity and ionicity of the glass network.

Overall, the TeO_2–BaO–V_2O_5 and TeO_2–V_2O_5–MoO_3 glasses exhibit high electronic polarizability, high optical basicity, and high refractive indices, combined with weak, mostly ionic bonding. These characteristics identify them as promising materials for nonlinear optical and photonic applications, with composition modification offering precise control over structure and optical performance.

1.4. Glasses in the systems Na_2O–CaO–SiO_2–Fe_2O_3, (Na_2O–CaO–SiO_2)/Fe_2O_3, and Na_2O–BaO–ZrO_2–TiO_2–SiO_2–B_2O_3–Al_2O_3

(Publications 6, 7, 8 of B4)

For Fe_2O_3-containing systems, it was established that homogeneous glasses are obtained up to 15 mol% Fe_2O_3, while at 20 mol%, partial crystallization occurs with the formation of magnetite (Fe_3O_4) and hematite (α-Fe_2O_3). Increasing Fe_2O_3 concentration leads to a rise in density, molar volume, and refractive index, along with changes in oxygen packing density, reflecting depolymerization of the silicate network.

FTIR spectra show distinct changes in the positions and intensities of bands corresponding to Si–O–Si symmetric and asymmetric stretching and Si–O bending vibrations. With increasing Fe_2O_3 content, these bands shift to lower frequencies, indicating the formation of non-bridging oxygens (NBOs) and the breaking of Si–O–Si bridges. Additional bands characteristic of Fe–O–Si mixed bonds were observed, confirming that Fe participates in the structure both as a network modifier and as a network former. Mössbauer spectroscopy corroborated the presence of Fe^{3+} and Fe^{2+} ions in tetrahedral and octahedral coordination.

In the Na_2O–BaO–ZrO_2–TiO_2–SiO_2–B_2O_3–Al_2O_3 system, up to 6 mol% BaO can be successfully replaced by ZrO_2, resulting in an increase in density, oxygen density, and refractive index, accompanied by a decrease in molar volume, indicating densification and enhanced cross-linking. The FTIR spectra display bands corresponding to Si–O–Si/O–B–O deformation and B–O–B/B–O–Si stretching vibrations, confirming the presence of BO_3, BO_4, and SiO_4 polyhedra interconnected in a compact structure. A distinct band at 570–580 cm^{-1}, typical of $BaTiO_3$, suggests the formation of a secondary crystalline phase.

With increasing ZrO_2 concentration, the hardness, elastic modulus, and crystallization temperature all increase, associated with the formation of a stronger and more stable 3D network due to the incorporation of Zr^{4+} in octahedral coordination.

The results reveal two contrasting structural effects:

- Fe_2O_3 promotes network depolymerization and structural loosening,
- ZrO_2 enhances network cross-linking and stabilization.

These findings demonstrate the possibility of tailoring the optical, structural, and mechanical properties of oxide glasses through the controlled introduction of modifying oxides.

2. Synthesis and Characterization of Bioactive Glasses and Glass-Ceramics

2.1. Bioactive Borate Glasses

(Publications 9 and 10, indicator Г7)

This group of studies, presented under group "G," focuses on the synthesis and characterization of bioactive borate glasses, carried out within the Department of Silicate Technology at the University of Chemical Technology and Metallurgy (UCTM). The research on the systems $CaO–Na_2O–B_2O_3–P_2O_5$ and $ZnO/MgO–CaO–Na_2O–B_2O_3–P_2O_5$ was conducted as part of a Scientific Research Fund project coordinated by Assist. Prof. Tina Tasheva. The candidate's main contribution involved glass synthesis and structural characterization.

Samples with identical compositions in the $B_2O_3–Na_2O–CaO–P_2O_5$ system were prepared by both melt-quenching and slow cooling, using porcelain and corundum crucibles. As a result, four distinct materials were obtained, depending on the crucible type and cooling rate.

X-ray diffraction (XRD) analysis showed that the corundum-crucible melt-quenched sample was almost completely amorphous, whereas the slow-cooled sample with the same composition exhibited near-complete crystallization. Samples prepared in porcelain crucibles were glass–ceramic, with two crystalline phases appearing during slow cooling. Scanning Electron Microscopy (SEM) revealed significant morphological and microstructural differences between slowly cooled samples prepared in different crucibles.

FTIR and Raman spectroscopy confirmed the presence of BO_3 and BO_4 units, likely connected in pentaborate superstructural groups. The results demonstrated that both the crucible material and cooling rate significantly influence the amorphous/crystalline structure and the formation of specific crystalline phases. In corundum crucibles, aluminum from the crucible was incorporated into the amorphous network, suppressing crystallization during rapid cooling and forming an AlP_3O_9 phase during slow cooling. In contrast, porcelain crucibles yielded $CaNa_3BO_{10}$ and α–$CaNaPO_4$ (renanite) crystalline phases.

The findings clearly indicate that while the phase composition depends on cooling and crucible conditions, the main structural units of the borate network remain BO_3 and BO_4, interconnected into pentaborate structures.

The second group of glasses, in the B_2O_3–Na_2O–CaO–P_2O_5 system modified with ZnO and MgO, was synthesized using the melt-quenching method. Physicochemical parameters indicated densities between 2.538–2.623 g/cm^3, molar volumes of 26.566–27.420 cm^3/mol, and oxygen packing densities of 73.669–76.262 mol/cm^3.

The incorporation of ZnO and MgO strongly influenced the structure and bonding within the glass network. When both modifiers were present, a decrease in density, an increase in molar volume, and a reduction in oxygen density were observed — indicating increased free volume and non-bridging oxygen (NBO) content. This corresponds to a lower degree of network connectivity.

FTIR and Raman spectroscopy revealed that the primary structural units are BO_3 and BO_4, connected by B–O–B linkages in pentaborate and pyroborate structural groups. The simultaneous presence of ZnO and MgO promoted the formation of triborate units.

These results confirm a strong correlation between composition and structural features, showing that the addition of ZnO and MgO leads to structural modification and partial depolymerization of the borate glass network, which can directly affect their bioactivity and dissolution behavior.

2.2. Bioactive Silicate and Borosilicate Glasses and Glass-Ceramics

(Publications 9 and 10, indicator B4)

This group of studies, presented under group “B,” focuses on the synthesis and characterization of bioactive silicate and borosilicate glasses and glass-ceramics. The work was performed by a research team at the Department of Silicate Technology, UCTM, including Assist. Prof. Tina Tasheva, as part of the national project BG-RRP-2.004-0002-C01 “BiOrgaMCT – Bioactive Organic and Inorganic Advanced Materials and Clean Technologies”, funded under the National Recovery and Resilience Plan. The candidate’s main role was the structural characterization of materials.

In the first study (publication 9, indicator B4), multicomponent glasses were designed as glaze coatings for dental zirconia ceramics (Y-TZP). The glasses were obtained by melting and rapid quenching, followed by grinding to <40 μm powders. To study crystallization tendencies, samples were thermally treated and analyzed by XRD and FTIR spectroscopy. The glass transition temperature (Tg), softening temperature (Ts), and coefficient of thermal expansion (CTE) were determined.

Selected glass compositions were applied as glazes on zirconia substrates and fired in a vacuum dental furnace. SEM analysis revealed homogeneous, crack-free, and pore-free coatings with excellent adhesion. The glass with the highest alkali oxide content exhibited a CTE closely matching zirconia, along with high transparency and good flowability, making it a promising candidate for dental applications.

In the second study (publication 10, indicator B4), a new bioactive glass-ceramic material was developed, based on biogenic hydroxyapatite (BHA) synthesized from *Rapana venosa* seashells, combined with monocalcium phosphate monohydrate. The compositions contained

SiO_2, B_2O_3, and Na_2O, and were prepared by melting and rapid quenching. Dense ceramic samples containing 25 wt.% glass (B_2O_3–SiO_2–Al_2O_3–Na_2O) were sintered.

XRD, FTIR, and SEM analyses revealed the coexistence of a crystalline hydroxyapatite phase ($Ca_{10}(PO_4)_6(OH)_2$) and an amorphous phase. Increasing SiO_2 content resulted in the formation of $Na_3Ca_6(PO_4)_5$ and a reduction in hydroxyapatite content. FTIR spectra confirmed the presence of SiO_4, PO_4, and BO_3 structural units, linked via Si–O–Si, B–O–B, P–O–P, and Si–O–Al bonds, which provide structural stability and bioactivity.

In vitro tests in simulated body fluid (SBF) demonstrated the formation of an apatite layer on the material surface, confirming its bioactive potential.

Both studies indicate that the synthesized glasses and glass-ceramics possess excellent adhesion, chemical compatibility, and bioactivity, making them highly suitable for dental and biomedical applications.

3. Electronic Polarizability and Group Optical Basicity

(Publications 1, 2, 3, 4, and 5, indicator B4)

This group of studies presents the candidate's contributions related to the determination of electronic polarizability and group optical basicity of simple oxides, binary, and ternary oxide glasses. The research was carried out jointly between the Department of Silicate Technology at UCTM (Bulgaria) and the Department of Materials Science and Technology at Nagaoka University of Technology (Japan).

Publications 1 and 2 from group "B" focus on the development of refined equations for calculating the optical basicity and average single bond strength (BM–O) of glasses from different oxide systems, including PbO–B_2O_3, Na_2O–B_2O_3, Na_2O–SiO_2, R_2O–RO–TeO_2, Bi_2O_3–B_2O_3, and ZnO–Bi_2O_3–B_2O_3. These equations take into account molar fractions and the group optical basicity of individual structural units. The concept of optical basicity, proposed by Duffy, is recognized as a key parameter in glass science and technology. For PbO–B_2O_3 glasses, equations were proposed that consider the molar fractions and group basicities of structural units such as BO_3, BO_4, PbO_3, PbO_4, and PbO_6. The calculations demonstrated that with increasing PbO content, the average bond strength decreases, while the optical basicity increases. This trend is attributed to the higher number of Pb–O–B and Pb–O–Pb bonds containing highly polarizable oxide ions. The variation of optical basicity $\Lambda(n_0)$ determined from refractive index data, and the theoretical optical basicity Λth(1), showed a similar dependence on PbO content, with a noticeable slope change near 50 mol% PbO, indicating a transition in the structural role of PbO.

The group (microscopic) optical basicity, introduced by Dimitrov and Komatsu based on the Duffy–Ingram model, was applied to binary and ternary tellurite glasses from the systems $R_2O(RO)$–TeO_2 and $10R_2O\cdot10R'O\cdot80TeO_2$ (where R = Li, Na, K; R' = Mg, Ba, Zn). The group optical basicity of different TeO_4 and TeO_3 units depends on the presence of non-bridging oxygens (NBOs): TeO_4 with one NBO → $\lambda = 1.23$; TeO_4 without NBO → $\lambda = 0.99$; terminal TeO_3 with two NBOs → $\lambda = 0.82$.

Equations were proposed for calculating Λth(1) and BM–O for various oxide glasses, considering the molar fractions of structural units such as BO_3, BO_4, SiO_4, GeO_4, GeO_6, PbO_3, PbO_4, and PbO_6. The analysis across different glass systems (borate, silicate, germanate, tellurite, and heavy-metal-oxide glasses) showed a general trend: increasing optical basicity corresponds to weaker average bond strength, reflecting higher oxide-ion polarizability and structural modifications in the glass network.

Publication 3 focuses on the electronic polarizability of Bi_2O_3-based glasses containing various oxides — classical glass formers (SiO_2, P_2O_5, GeO_2, B_2O_3), conditional formers (TeO_2), network modifiers (Li_2O, ZnO), and other oxides (PbO, Ga_2O_3, RE_2O_3).

For these systems, optical basicity ($\Lambda(n_0)$) and the interionic interaction parameter ($A(n_0)$) were calculated using equations derived from the Lorentz–Lorenz formula and Yamashita–Kurosawa theory. The analysis revealed a strong correlation between $\Lambda(n_0)$ and $A(n_0)$ in Bi_2O_3-based glasses: as Bi_2O_3 content increases, $\Lambda(n_0)$ increases while $A(n_0)$ decreases, indicating enhanced electronic polarizability and weaker bonding. When compared to other glass systems lacking Bi_2O_3 (e.g., B_2O_3–SiO_2, $Li_2O/Na_2O/ZnO$–$B_2O_3/SiO_2/P_2O_5$, Li_2O/Na_2O–GeO_2, and $Li_2O/Na_2O/ZnO$–TeO_2), Bi_2O_3-based glasses exhibited exceptionally high optical basicity ($\Lambda(n_0) \approx 1.15$) and very low interionic interaction parameter ($A(n_0) \approx 0.01$ Å^{-3}). For comparison, TeO_2-based glasses have $\Lambda(n_0) \approx 1.0$ and $A(n_0) \approx 0.03$ Å^{-3}.

These features explain the unique properties of Bi_2O_3-rich glasses, such as: ability to reduce to lower valence states, low glass transition temperatures (Tg ≈ 232 °C) for nearly pure Bi_2O_3 glass, brittle character and low phonon energy, high third-order nonlinear optical susceptibility, and capacity to form functional RE^{3+}-doped crystalline phases.

In publication 4, the optical basicity $\Lambda(n_0)$ of selected binary and ternary silicate glasses was determined using the Lorentz–Lorenz relation based on refractive index data. Comparing the experimentally determined optical basicity (Λexp) with the theoretical value (Λth) provided deeper insight into the electronic polarizability and the structural roles of glass formers, intermediates, and network modifiers.

A new set of optical basicity values for individual oxides was proposed, improving the quantitative correlation between optical basicity and glass composition. Examples include: $\Lambda(SiO_{2}\_glass) = 0.53$ (higher than the conventional $\Lambda(SiO_{2}\_oxide) = 0.48$), $\Lambda(Al_2O_{3}\_glass) = 0.62$, $\Lambda(TiO_{2}\_glass) = 1.04$.

This study highlights the relationship between optical basicity and oxide coordination structures in silicate glasses, showing that comparison between $\Lambda(n_0)$ and Λth serves as an effective tool for quantitatively assessing electronic polarizability in glass systems.

Publication 5 analyzes the structural role of Nb_2O_5 in multicomponent oxide glasses, particularly K_2O–Nb_2O_5–SiO_2 with high Nb_2O_5 content (>10 mol%). The presence of weakly and strongly distorted NbO_6 octahedra, as well as the formation of Nb–O–Nb and Nb–O–Si/B/Ge/P/Te bonds, plays a critical role in determining glass properties.

Nb_2O_5 typically acts as a glass-forming oxide, establishing covalent bonds with other structural units and stabilizing the glass network. Weakly distorted NbO_6 octahedra, characterized by low phonon energy (~600 cm^{-1}) and the clustering of corner-shared Nb_2O_5 octahedra, enhance the electronic polarizability and improve the optical performance of rare-earth ions.

Nb_2O_5-rich regions promote nanoscale compositional fluctuations, facilitating nucleation and growth of functional nanocrystals, such as $LiNbO_3$ and $Sr_xBa_{1-x}Nb_2O_6$.

The discussed structural and bonding characteristics of Nb_2O_5 provide valuable insights for designing new functional oxide glasses and glass-ceramics containing niobium, with enhanced electrical and optical properties.

5. Characterization of carbonation products of cement kiln dust.

(publication 8 from indicator G7)

In this group, the candidate presents a study from group “G” related to the characterization of carbonation products of cement kiln dust. This research topic was developed by a team from the Institute of Mineralogy and Crystallography at the Bulgarian Academy of Sciences (BAS). The studies under this point were carried out as part of a project funded by the National Science Fund, with Assistant Professor Tina Tasheva being a member of the research team. The main contribution of the candidate was related to the structural characterization of the materials.

Cement kiln dust is a by-product of clinker production, rich in alkaline and alkaline earth compounds, which makes it suitable for capturing CO_2 through mineral carbonation. The study examined two approaches: direct carbonation of dry dust and carbonation of hydrated dust.

The infrared analysis of the studied materials and their carbonated forms showed a clear distinction between the structures before and after carbonation. The spectra of the untreated samples exhibited complex bands characteristic of silicate, sulfate, and hydrated phases, including vibrations of SiO_4 and SO_4 structural groups, as well as the presence of chemically bound water. In contrast, the spectra of the samples after carbonation displayed well-defined bands characteristic of the CO_3 structural unit, confirming the formation of calcite. The disappearance of bands associated with hydrated phases was also observed, along with weak traces of vaterite.