Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

Fakulteta za kemijo in kemijsko tehnologijo / Faculty of chemistry and chemical technology

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Miha Lukšič, miha.luksic@fkkt.uni-lj.si

3. Raziskovalno področje (*Research field*):

Kemija (fizikalna kemija) / Chemistry (physical chemistry)

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Slov.: Usposabljanje mladega raziskovalca bo potekalo v okviru doktorskega študijskega programa Kemijske znanosti na Fakulteti za kemijo in kemijsko tehnologijo Univerze v Ljubljani. Mladi raziskovalec bo vključen v raziskovalno dejavnost programske skupine Fizikalna kemija (P1-0201). Kandidat bo med študijem opravil predpisane obvezne in izbirne študijske obveznosti, oblikoval temo doktorske disertacije, izvedel raziskovalno delo na izbranem področju ter pripravil in uspešno zagovarjal doktorsko disertacijo. Raziskovalno delo bo s področja fizikalne kemije in bo osredotočeno na razumevanje molekulskih interakcij v vodnih raztopinah (zlasti elektrolitov in polielektrolitov). Vključevalo bo kombinacijo teoretične kemije (kvantna kemija, statistična termodinamika), računalniških simulacij (molekulska dinamika, simulacije Monte Carlo), strojnega učenja ter eksperimentalnega dela. Kandidat bo imel med študijem priložnost udeležiti se mednarodnih konferenc in opraviti del svojega raziskovalnega dela v tujini. Od kandidata se pričakuje aktivno znanje angleškega jezika, poznavanje osnov fizikalne kemije, molekulskega modeliranja, programiranja ter eksperimentalne spretnosti (npr. priprava raztopin, izvajanje fizikalno-kemijskih meritev).

Eng.: The training of the young researcher will take place within the doctoral study programme in Chemical Sciences at the Faculty of Chemistry and Chemical Technology, University of Ljubljana. The young researcher will be integrated into the research activities of the Physical Chemistry research programme group (P1-0201). During the course of study, the candidate will complete the required compulsory and elective coursework, define the topic of the doctoral dissertation, conduct research in the selected field, and prepare and successfully defend the doctoral thesis. The research will be in the field of physical chemistry, focusing on understanding molecular interactions in aqueous solutions (particularly electrolytes and polyelectrolytes). It will involve a combination of theoretical chemistry (quantum chemistry, statistical thermodynamics), computer simulations (molecular dynamics, Monte Carlo simulations), machine learning, and experimental work. During the PhD studies, the candidate will have the opportunity to attend international conferences and carry out part of the research abroad. The candidate is expected to have an active command of English, a solid background in physical chemistry, knowledge of molecular modelling and programming, as well as basic experimental skills (e.g. preparation of solutions and performing physicochemical measurements).

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***

- kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja)
  (candidate who has completed a Master's degree (2nd Bologna level)):
  - diplomska listina / potrdilo o zaključku študijskega programa
    (diploma certificate / certificate of completion of the study programme)
  - priloga k diplomi / potrdilo o opravljenih obveznostih
    (diploma supplement / official transcript of records containing all grades obtained in the study programme)
- kandidat, ki še ni zaključil študija na 2. stopnji

(candidate who has not yet completed a Master's degree):

- potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
  (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☐ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☒ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☒ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☐ **osnutek idejne zasnove raziskovalnega dela** *(preliminary research proposal)*

☐ **priporočilno pismo** *(letter of recommendation)*

☐ **druge priloge** *(other attachments):*

Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

Fakulteta za kemijo in kemijsko tehnologijo (FKKT)

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

izr. prof. dr. Miha Pavšič (miha.pavsic@fkkt.uni-lj.si)

3. Raziskovalno področje (*Research field*):

1.05 Biokemija in molekularna biologija

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Slov.: Kandidat_ka bo preučeval_a organizacijo in regulacijo aktinskega citoskeleta v širšem evolucijskem in mehanističnem kontekstu z integracijo biofizike in strukturne biologije. Osrednji cilj raziskave je razkriti molekularna načela, ki uravnavajo tvorbo (višjerednih) na filamentih osnovanih struktur. Poseben poudarek bo namenjen preučevanju interakcij med aktinskimi filamenti in njihovimi regulatornimi partnerji, na primer povezovalnimi proteini (prečnimi povezovalci) ter modulacijskimi proteini, ki skupaj oblikujejo arhitekturo in dinamiko citoskeleta. Z uporabo kombinacije in vitro rekonstitucije, biofizikalnih meritev ter visokoločljivostnih strukturnih pristopov, kot so rentgenska kristalografija, krio-elektronska mikroskopija in sipanje v raztopini, bo kandidat_ka analiziral_a, kako regulatorni dejavniki nadzorujejo obnašanje filamentov na molekularni in supramolekularni ravni. V dopolnilni smeri se bo projekt razširil na manj raziskane citoskeletne sisteme z namenom preučevanja funkcionalne diverzifikacije znotraj aktinske superdružine. Primerjalne biokemijske in strukturne analize bodo omogočile prepoznavanje ohranjenih in divergentnih regulatornih mehanizmov ter prispevale k razumevanju, kako se aktinski polimeri prilagajajo različnim celičnim kontekstom. Od kandidata_ke se pričakuje obvladanje osnov bioinformatike in strukturne biologije.

Eng.: The candidate will investigate the organization and regulation of the actin cytoskeleton in a broad evolutionary and mechanistic context, integrating biophysics and structural biology. The primary objective is to uncover molecular principles that govern filament (higher-order) assembly. Particular emphasis will be placed on the interplay between actin filaments and their regulatory partners, for example crosslinkers, and modulatory proteins that collectively shape cytoskeletal architecture and dynamics. Using a combination of in vitro reconstitution, biophysical measurements, and high-resolution structural approaches such as X-ray crystallography, cryo-electron microscopy and solution scattering, candidate will dissect how regulatory factors control filament behavior at molecular and supramolecular levels. In a complementary direction, the project will extend to less-characterized cytoskeletal systems to explore functional diversification within the actin superfamily. Comparative biochemical and structural analyses will identify conserved and divergent regulatory mechanisms, providing insight into how actin-based polymers adapt to distinct cellular contexts. The candidate is expected to have a working knowledge of the fundamentals of bioinformatics and structural biology.

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***
− kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja) *(candidate who has completed a Master's degree (2nd Bologna level)):*
o diplomska listina / potrdilo o zaključku študijskega programa *(diploma certificate / certificate of completion of the study programme)*
o priloga k diplomi / potrdilo o opravljenih obveznostih *(diploma supplement / official transcript of records containing all grades obtained in the study programme)*
− kandidat, ki še ni zaključil študija na 2. stopnji

(candidate who has not yet completed a Master's degree):

- potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
  (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☐ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☐ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☒ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☐ **osnutek idejne zasnove raziskovalnega dela** *(preliminary research proposal)*

☐ **priporočilno pismo** *(letter of recommendation)*

☐ **druge priloge** *(other attachments):*

Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

Univerza v Ljubljani, Fakulteta za kemijo in kemijsko tehnologijo University of Ljubljana, Faculty of Chemistry and Chemical Technology

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Doc. Dr. Nejc Petek, nejc.petek@fkkt.uni-lj.si

3. Raziskovalno področje (*Research field*):

1.04 Kemija (1.04.04 Organska kemija) 1.04 Chemistry (1.04.04 Organic chemistry)

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Uvod:
Fotoredoks kataliza se je uveljavila kot metoda v organski sintezi, ki poteka pod blagimi reakcijskimi pogoji in jo je, glede na uporabljeni katalizator in reagente, mogoče obravnavati kot okolju prijazno. Ker običajno poteka prek radikalnih intermediatov, omogoča transformacije organskih spojin, ki bi jih sicer težko dosegli zgolj s termičnimi pretvorbami. Čeprav se fotoredoks kataliza uporablja za tvorbo številnih različnih vezi, ponuja tvorba vezi C–S možnosti za sintezo tiolov, sulfonov, sulfonamidov, sulfonil fluoridov in drugih žveplovih spojin s pomočjo fotoredoks katalize.

Izhodišče in okvir raziskave:
V osredju projekta bo uporaba fotoredoks katalize za tvorbo C–S vezi. Za sintezo izhodnih spojin, derivatizacijo produktov ter sintezno podporo bodo uporabljene tudi druge metode. Naloge raziskovalca ali raziskovalke (v nadaljevanju se moška slovnična oblika uporablja za oba spola) bodo obsegale delo na področju organske sinteze, kot so presejalne testne reakcije, optimizacija reakcijskih pogojev, preučevanje nabora substratov, mehanistične študije ter merjenje fizikalnih in drugih potencialnih lastnosti ali uporabnosti spojin, na primer biološke aktivnosti.

Umestitev v raziskovalni program ali projekt:
Raziskovalno delo bo potekalo v okviru programske skupine P1-0179 (Napredna organska sinteza in kataliza, vodja: prof. dr. Jurij Svete).

Cilji:
Cilj raziskave bodo:
-sinteza ustreznih substratov z uporabo obstoječih in novih metod,
-razvoj novih sinteznih metod za pripravo organskih spojin, ki vsebujejo žveplo, s poudarkom na transformacijah, kataliziranih s fotoredoks katalizo,
-primerjava razvitih metod z obstoječimi glede na število potrebnih korakov, varnost, uporabnost, vpliv na okolje, stroške, nabor produktov in druge parametre,
-preučevanje reakcijskih mehanizmov,
-določanje lastnosti sintetiziranih spojin,
-uporaba žveplovih spojin pri sintezi novih heterocikličnih spojin,
-testiranje biološke aktivnosti sintetiziranih spojin ter njihova uporaba v biokonjugaciji v širšem interdisciplinarnem okviru.

Metode:
V okviru projekta bo raziskovalec uporabljal vse sodobne preparativne in izolacijske metode ter tehnike organske sinteze. Struktura produktov bo določena s spektroskopskimi metodami (IR, MS, HRMS; ^{1}H NMR, ^{13}C NMR, 2D NMR itd.), analitskimi metodami (CHN analiza, LC-MS) in rentgensko difrakcijo. Reakcijski mehanizmi bodo raziskani z eksperimentalnimi in računalniškimi metodami. Biološka aktivnost in potencial za biokonjugacijo bosta ovrednotena na ustreznih peptidih in proteinih, metode pa bodo ocenjene z ustreznimi analitskimi postopki v biokemiji.

Od kandidata za delovno mesto se pričakuje teoretično in praktično znanje s področja organske sinteze in analize.

Introduction:
Photoredox catalysis has emerged as a method in organic synthesis that takes place under mild reaction conditions and can, depending on the catalyst and reagents used, be considered environmentally firendly. Moreover, as it usually proceedes via radical intermediates, it enables transformations of organic compounds which would otherwise be difficult to achieve using only thermal conversions. While photoredox catalysis has been utilized for the construction of numerous different bonds, the C–S bond construction offers opportunities to utilize photoredox catalysis in the synthesis of thiols, sulfones, sulfonamides, sulfonyl fluorides and other sulfur compounds.

Starting point and framework of the work program:
The focal point of the project will be the use of photoredox catalysis for the construction of C–S bonds. Other methods will also be used for the synthesis of starting materials, derivatization of products and as complimentary methods. Researcher's tasks will include those in organic synthesis, such as initial screening of reactions, optimization of reaction conditions, substrate scope, mechanistic studies, as well as measuring physical and other potential properties or utilizations of compounds, such as biological activities.

Placement in the research program or project:
The research work will be carried out within the program group P1-0179 (Advanced organic synthesis and catalysis, leader: Prof. Dr. Jurij Svete).

Objectives:
The aim of the research will be to:
- synthesis of suitable substrates using existing and novel methods,
- development of novel synthetic methods towards sulfur-containing organic compounds with the focus on photoredox-catalyzed transformations,
- comparison of developed methods to the existing ones in respect to the number of required steps, safety, applicability, environmental impact, cost, scope and other parameters,
- study of reaction mechanisms,
- determination of the properties of the synthesized compounds,
- utilization of sulfur-compounds in the synthesis of novel heterocyclic compounds,
- testing for biological activity of synthesized compounds and their use in bioconjugation within a broader interdisciplinary framework.

Methods:
As part of the project, the researcher will apply all modern preparative-isolation methods and techniques of organic synthesis. The structure of the products will be determined using spectroscopic methods (IR, MS, HRMS; ^{1}H NMR, ^{13}C NMR, 2D NMR, etc.), analytical methods (CHN analysis, LC-MS) and X-ray diffraction. The reaction mechanisms will be investigated using both experimental and computational methods. The biological activity and potential in bioconjugation will be measured on appropriate peptides and proteins and the evaluation of the methods conducted using appropriate analytical methods in biochemistry.

An applicant for the position is expected to have theoretical and practical knowledge in the field of organic synthesis and analysis.

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***

- kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja)
  (candidate who has completed a Master's degree (2nd Bologna level)):
  - diplomska listina / potrdilo o zaključku študijskega programa
    (diploma certificate / certificate of completion of the study programme)
  - priloga k diplomi / potrdilo o opravljenih obveznostih
    (diploma supplement / official transcript of records containing all grades obtained in the study programme)
- kandidat, ki še ni zaključil študija na 2. stopnji
  (candidate who has not yet completed a Master's degree):
  - potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
    (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☒ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☒ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☐ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☐ **osnutek idejne zasnove raziskovalnega dela** *(preliminary research proposal)*

☐ **priporočilno pismo** *(letter of recommendation)*

☐ **druge priloge** *(other attachments):*

Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

Fakulteta za kemijo in kemijsko tehnologijo (*Faculty of Chemistry and Chemical Technology*)

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Marta Počkaj; marta.pockaj@fkkt.uni-lj.si

3. Raziskovalno področje (*Research field*):

Anorganska kemija (*Inorganic Chemistry*)

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Slov.: *Usposabljanje mladega raziskovalca bo potekalo v okviru raziskovalnega programa P1-0175 Napredna anorganska kemija. Kandidat se bo pri svojem raziskovalnem delu osredotočil na določanje kristalnih struktur izbrane skupine materialov z zanimivimi kemijskimi, biološkimi in/ali fizikalnimi lastnostmi. Določitev kristalne strukture snovi je namreč izjemnega pomena, saj s poznavanjem položaja in načina povezovanja gradnikov lahko razlagamo in napovedujemo od nje odvisne kemijske, fizikalne in druge lastnosti snovi. Kandidat se bo usposobil za delo v sodobno opremljenem difrakcijskem laboratoriju, pri čemer se bo spoznal z različnimi difrakcijskimi tehnikami (elektronska difrakcija, rentgenska difrakcija na monokristalu, rentgenska praškovna difrakcija) ter prednostmi in omejitvami posameznih metod. Seznanil se bo tudi z ostalimi spektroskopskimi in analitskimi tehnikami, primernimi za karakterizacijo izbrane skupine materialov.* *Kandidat mora izkazati zelo dobro pisno in govorno znanje angleščine, zelo dobro pisno in govorno znanje slovenskega jezika ali se zavezati, da se ga nauči. Kandidat mora biti ustvarjalen in inovativen ter imeti visoko stopnjo motivacije za samostojno delo v laboratoriju kot tudi v skupini. Usposabljal se bo za pisanje člankov in predstavitev na mednarodnih konferencah.*

Eng.: *The training of the young researcher will take place within the framework of the research program P1-0175 Advanced Inorganic Chemistry. In the research work, the candidate will focus on determination of crystal structures of a selected group of materials with interesting chemical, biological and/or physical properties. Crystal structure determination of a substance is of utmost importance, since by knowing the position of the atoms and the way of the building blocks connect, we can explain and predict the chemical, physical and other properties of the substance that depend on it. The candidate will be trained to work in a modern equipped diffraction laboratory, where he/she will become familiar with various diffraction techniques (electron diffraction, single-crystal X-ray diffraction, X-ray powder diffraction) and the advantages and limitations of individual methods. He/She will also become familiar with other spectroscopic and analytical techniques suitable for the characterization of the selected group of materials. The candidate must demonstrate very good written and spoken English, very good written and spoken Slovenian or be committed to learning it. The candidate must be creative and innovative and have a high*

level of motivation for independent work in the laboratory as well as in a group. He/she will be trained in writing articles and presenting at international conferences.

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***

- kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja)
  (candidate who has completed a Master's degree (2nd Bologna level)):
  - diplomska listina / potrdilo o zaključku študijskega programa
    (diploma certificate / certificate of completion of the study programme)
  - priloga k diplomi / potrdilo o opravljenih obveznostih
    (diploma supplement / official transcript of records containing all grades obtained in the study programme)
- kandidat, ki še ni zaključil študija na 2. stopnji
  (candidate who has not yet completed a Master's degree):
  - potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
    (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☐ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☒ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☐ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☐ **osnutek idejne zasnove raziskovalnega dela** *(preliminary research proposal)*

☒ **priporočilno pismo** *(letter of recommendation)*

☐ **druge priloge** *(other attachments):*

Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

Fakulteta za kemijo in kemijsko tehnologijo UL

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Helena Prosen, helena.prosen@fkkt.uni-lj.si

3. Raziskovalno področje (*Research field*):

Analizna kemija, Kemija okolja

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Slov.: Človeške dejavnosti povzročajo vnos številnih sintetskih spojin v okolje, kjer jih obravnavamo kot onesnaževala (kontaminante, polutante). Večina jih je biološko aktivnih in pri organizmih v okolju, ravno tako tudi pri človeku, povzročajo različne fiziološke odzive od blagih motenj do izrazito toksičnih učinkov. Poleg tega so spojine po vnosu v okolje lahko podvržene različnim procesom, zlasti pomembna sta biotski in abiotski razkroj, pri čemer nastajajo nove spojine z neznanimi učinki. Koncentracijo onesnaževal ter njihovih razgradnih produktov je nujno spremljati v različnih delih okolja, da lahko ugotovimo, kaj se z njimi dogaja. Posebej pomembna skupina onesnaževal so t. im. emergentna ali novodobna onesnaževala (angl. *contaminants of emerging concern*, CEC), za katere je značilno, da povečini zanje še ne obstajajo zakonske meje glede izpustov in tudi njihovi učinki na žive organizme še niso docela raziskani. Program usposabljanja mlade-ga raziskovalca/-ke bo zajemal razvoj različnih tehnik priprave (ekstrakcijske in mikroekstrakcijske tehnike) in analize vzorcev (plinska in tekočinska kromatografija v povezavi s tandemsko ali visokoločljivostno masno spektrometrijo, površinske tehnike analize) za izbrana novodobna onesnaževala v različnih delih okolja, kjer se običajno nahajajo v zelo nizkih koncentracijah. Preučeval-a bo obnašanje in morebitno razgradnjo izbranih onesnaževal pri normalnih in ekstremnejših okoljskih pogojih, kakršne bi morda lahko pričakovali med bolj izraženimi podnebnimi spremembami. Predvidoma bo identificiral-a pretvorbene produkte in ovrednotil-a njihovo škodljivost v okolju z *in silico* ter *in vitro* metodami. Zaželeno je, da ima kandidat-ka dobra kemijska ali sorodna naravoslovna znanja, predvsem na področju eksperimentalne analizne kemije. Poleg tega se pričakuje osnovno poznavanje kemijskih procesov v okolju. Nujno je dobro znanje angleškega jezika. Pri prijavi na razpis naj kandidat-ka priloži kratek opis (največ ena stran) razlogov in motivacije, zakaj bi želel-a raziskovati na področju opisane tematike.

Eng.: Human activities cause the introduction of numerous synthetic compounds into the environment, which are considered pollutants (contaminants). Most of them are biologically active and cause various physiological responses in organisms in the environment, including humans, ranging from mild disturbances to highly toxic effects. In addition, compounds can undergo various processes after entering the environment, of particular importance being biotic and abiotic degradation, which result in the formation of new compounds with unknown effects. It is essential to monitor the concentration of pollutants and their degradation products in different parts of the environment in order to determine what is happening to them. A particularly important group of pollutants are

the so-called emerging pollutants (i.e., contaminants of emerging concern, CEC), which are characterized by the fact that most of them do not yet have legal limits on emissions and their effects on living organisms have not yet been fully investigated.

The training programme for the young researcher will cover the development of various sample preparation techniques (extraction and microextraction techniques) and sample analysis (gas and liquid chromatography coupled to tandem or high-resolution mass spectrometry, surface analysis techniques) for selected emerging pollutants in various parts of the environment, where they are usually found in very low concentrations. The behaviour and possible degradation of selected pollutants under normal and more extreme environmental conditions, such as might be expected during more pronounced climate change, will be studied. It is expected that the young researcher will identify transformation products and evaluate their environmental harmfulness using *in silico* and *in vitro* methods.

It is desirable that the candidate has good knowledge of chemistry or related natural sciences, especially in the field of experimental analytical chemistry. In addition, basic knowledge of chemical processes in the environment is expected. Good knowledge of the English language is essential. When applying for the call, the candidate should attach a short description (maximum one page) of the reasons and motivation why he/she would like to research in the area of the described topic.

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***

- kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja)
  (candidate who has completed a Master's degree (2nd Bologna level)):
  - diplomska listina / potrdilo o zaključku študijskega programa
    (diploma certificate / certificate of completion of the study programme)
  - priloga k diplomi / potrdilo o opravljenih obveznostih
    (diploma supplement / official transcript of records containing all grades obtained in the study programme)
- kandidat, ki še ni zaključil študija na 2. stopnji
  (candidate who has not yet completed a Master's degree):
  - potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
    (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☒ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☒ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☒ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☒ **osnutek idejne zasnove raziskovalnega dela: napišite svoje ideje znotraj predlaganega opisa s strani mentorice** *(preliminary research proposal: write your ideas within the proposed description by the mentor)*

☒ **priporočilno pismo – samo kandidati, ki niso z UL FKKT** *(letter of recommendation – only candidates other than from UL FKKT)*

☐ **druge priloge** *(other attachments):*

Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

Fakulteta za kemijo in kemijsko tehnologijo

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Tjaša Rijavec, Tjasa.Rijavec@fkkt.uni-lj.si

3. Raziskovalno področje (*Research field*):

Analizna kemija

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Slov.: *Tematika raziskovalnega dela bo osredotočena na analizo proteinskih materialov kulturne dediščine, kot npr. svila, pergament, usnje, ter proteinski ostanki na arheološki keramiki. Takšni materiali so zelo raznoliki in vsebujejo informacije o izvoru materiala, tehnoloških postopkih izdelave in procesih dolgoročnega staranja.* *Glavni del raziskav bo osredotočen na proteomiko na osnovi masne spektrometrije, ki omogoča poglobljeno karakterizacijo z identifikacijo proteinov ter preučevanje razgradnih sprememb. Eden od pristopov je bottom-up analiza po encimski razgradnji proteinov na peptide (LC-MS/MS), raziskane pa bodo tudi možnosti analize proteinov v nativni obliki. Proteinske materiale se lahko analizira tudi z velikostnoizključitveno kromatografijo (SEC) sklopljeno z detektorjem na sipanje svetlobe (MALS), za določanje porazdelitve molske mase. Del raziskave bo namenjen tudi razvoju minimalno porušnih pristopov vzorčenja v sledovih za muzejske predmete. Doktorska raziskava bo potekala na sodobnih analiznih tehnikah, kot so LC-MS, LC-MS/MS, DESI-MS, SEC-MALS.*

Eng.: *The topic of the research will focus on the analysis of proteinaceous materials in cultural heritage, such as silk, parchment, leather, and protein residues on archaeological ceramics. These materials are highly diverse and contain valuable information on the origin of the raw materials, manufacturing technologies, and long-term ageing processes.* *The main part of the research will focus on mass spectrometry-based proteomics, enabling in-depth characterization through the identification of proteins and the investigation of degradation-related modifications. One approach will involve bottom-up proteomics following enzymatic digestion of proteins into peptides (LC-MS/MS), while possibilities for native protein analysis will also be explored. Proteinaceous materials may additionally be analysed using size-exclusion chromatography (SEC) coupled with multi-angle light scattering (MALS) to determine molar mass distribution. Part of the research will also be devoted to the development of minimally invasive micro-sampling approaches for museum objects. The doctoral project will involve work with advanced analytical techniques, including LC-MS, LC-MS/MS, DESI-MS, and SEC-MALS.*

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***

- kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja)
  (candidate who has completed a Master's degree (2nd Bologna level)):

  - diplomska listina / potrdilo o zaključku študijskega programa
    (diploma certificate / certificate of completion of the study programme)

  - priloga k diplomi / potrdilo o opravljenih obveznostih
    (diploma supplement / official transcript of records containing all grades obtained in the study programme)

- kandidat, ki še ni zaključil študija na 2. stopnji
  (candidate who has not yet completed a Master's degree):

  - potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
    (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☐ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☒ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☒ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☐ **osnutek idejne zasnove raziskovalnega dela** *(preliminary research proposal)*

☐ **priporočilno pismo** *(letter of recommendation)*

☐ **druge priloge** *(other attachments):*

Opis raziskovalnega dela *(Research work description*)

1. Članica UL (*UL member)*:

UL FKKT

2. Ime, priimek in elektronski naslov mentorja/ice (*Mentor's name, surname and email*):

Andraž Šuligoj, andraz.suligoj@fkkt.uni-lj.si

3. Raziskovalno področje (*Research field*):

Anorganska kemija

4. Opis raziskovalnega dela *(Research work description*):
Vključuje morebitne dodatne pogoje, ki jih mora izpolnjevati kandidat/ka za mladega raziskovalca/ko, ki niso navedeni v razpisu za mlade raziskovalce *(It includes any additional conditions that the candidate for a young researcher must meet, which are not listed in the call to tender for young researchers.)*.

Slov.:

Filmi plastovitih dvojnih hidroksidov in kovinskih oksidov za fotokatalitsko zmanjševanje hlapnih organskih spojin in odstranjevanje farmacevtskih izdelkov

PREGLED RAZISKAV

Delo bo vključevalo razvoj večfunkcionalnih fotokatalitskih filmov, ki združujejo Zn–Al plasti dvojnih hidroksidov (LDH) s kovinskimi oksidi (TiO_2, ZnO, CuO) za dvojne aplikacije: (1) zmanjševanje hlapnih organskih spojin (VOC; formaldehid, toluen) in (2) odstranjevanje farmacevtskih onesnažil v vodi (naproksen, diklofenak, ibuprofen, sulfametoksazol) pod UV in kasneje sončno svetlobo. Ta združena platforma izkorišča dejstvo da se LDH-ji ponašajo z izjemno adsorpcijo onesnaževal, medtem ko LDH-ji kažejo tudi dobro fotokatalitsko aktivnost, kar v kombinaciji z oksidi omogoča prilagajanje materialov za specifično uporabo.

UTEMELJITEV IZBIRE MATERIALOV

Karbonatni-LDH zagotavlja visoko specifično površino bogato s hidroksili za močno adsorpcijo onesnaževal, kar je idealno za VOC ali farmacevtskih učinkovin. Kloridni-LDH pa kaže visoko fotokatalitsko aktivnost (morda preko kisikovih praznin ali reaktivnih klorovih zvrsti). Vključitev CuO, ki absorbira vidno svetlobo (npr. ~1,2–1,7 eV) skupaj s TiO_2 ali ZnO, ustvarja p-n heterospoje s kaskadnim prenosom naboja, kar razširja spektralni odziv čez modro-rdečo valovno dolžino in hkrati zatira rekombinacijo.

ZMANJŠANJE VOC (UPORABA V PLINSKI FAZI)

Onesnažila pri koncentracijah ppb–ppm v notranjem zraku zahtevajo močno adsorpcijo na plasti z visoko površino, ki ji sledi fotokatalitska mineralizacija v CO_2 in H_2O. Kompoziti LDH-oksid zagotavljajo dvojno funkcionalnost: Si–OH in Al–OH mesta adsorbirajo polarne VOC (npr. formaldehid) preko H-vezi ter aromatske spojine (npr. benzen, toluen) preko π-π zlaganja, medtem ko oksidni nanodelci fotooksidirajo adsorbirane snovi pod svetlobo. p-n heterospoj prostorsko ločuje nosilce naboja, s čimer podaljšuje življenjsko dobo in kvantno učinkovitost. Porozne plasti (2–50 μm) maksimirajo adsorpcijo katalizatorjev, medtem ko hierarhična poroznost (mikropore za površino, mezopore za transport, makropore za pretok plina) zagotavlja dostop onesnaževal skozi celotno globino filma.

ODSTRANITEV FARMACEVTSKIH UČINKOVIN (UPORABA V VODNI FAZI)

Farmacevtska mikroonesnaževala pri koncentracijah ng/L–μg/L zahtevajo predkoncentracijo preko adsorpcije na fotokatalitske plasti v reaktorjih s pretokom. Adsorpcija, odvisna od speciacije (anionski farmacevtski izdelki se pri pH 5–7 adsorbirajo na pozitivno nabite LDH površine preko elektrostatike in interakcij π-π) povzroči koncentracijo

onesnaževala blizu fotokatalitskih aktivnih mest. Osvetljevanje z ustrezno energijo ustvarja pare e^-/h^+; Luknje oksidirajo farmacevtska zdravila ali ustvarjajo ·OH, medtem ko elektroni reducirajo O_2 na $\cdot O_2^-$. Popolna mineralizacija v CO_2 (potrjena z analizo TOC in odsotnost strupenih intermediantov prek LC-MS) preprečuje kopičenje nezaželenih produktov. Vključitev TiO_2 omogoča dodatno UV absorpcijo in močno oksidirajoče luknje (+3,1 V v primerjavi z NHE), ki lahko napadejo stabilne aromatske obroče. Napredne konfiguracije materialov, npr. kombinacija karbonat-LDH-CuO (adsorpcija) s kloridom-LDH-CuO (hitra fotokataliza), optimizirajo splošno učinkovitost odstranjevanja.

IZDELAVA FILMOV

Filmi se pripravijo preko različnih tehnik: doctor-blade, tehnika potapljanja-vleke, tehnika pršenja, nato pa so toplotno obdelani pri 200–400 °C, da se LDH razgradi v mešane kovinske okside, pri čemer se ohrani hierarhična poroznost zaradi evolucije karbonatov/kloridov. Steklene, kovinske ali keramične podlage pa omogočajo različne toplotne obremenitve in možnosti v vgradnjo različnih reaktorjev.

MEHANISTIČNE ŠTUDIJE IN OPTIMIZACIJA

Poravnava pasov na heterospojih LDH-oksida (tip II proti Z-shemi) bo pojasnjena z naprednimi fotoluminiscenčnimi meritvami, foto-meritvami in spektroskopijo elektrokemijske impedance za optimizacijo ločevanja nabojev. Eksperimenti z radikalnim odstranjevanjem (tert-butanol za ·OH, benzokinon za $\cdot O_2^-$, EDTA za h^+) identificirajo dominantne reaktivne kisikove vrste. Kvantifikacija intermediatov preko LC-MS pokaže najbolj primerne materiale z najboljšim vplivom na okolje preko končnih produktov (popolna oksidacija do CO2 in H2O, spremljana z TOC analizo).

VPLIV

Uspešen razvoj takih plasti je lahko kasneje uporavljen v: (1) integraciji HVAC za neprekinjeno čiščenje zraka v notranjih prostorih, (2) fasadne premaze za zunanje zmanjševanje VOC, (3) reaktorje za čiščenje vode s pretokom za odstranjevanje farmacevtskih onesnažil v decentraliziranih sistemih.

KLJUČNE INOVACIJE:

(1) Dvojna funkcionalnost z izbiro LDH karbonata proti kloridu; (2) aktivnost vidne svetlobe preko integracije CuO in heterospojev p-n; (3) hierarhična poroznost, ki ohranja visoko površino v debelih plasteh; (4) razširljive metode premazov, združljive z industrijsko proizvodnjo; (5) enotna platforma za reševanje onesnaženja zraka in vode s skupnim fotokatalitskim mehanizmom.

Eng.:

Films of layered double hydroxides and metal oxides for photocatalytic reduction of volatile organic compounds and removal of pharmaceutical products

RESEARCH OVERVIEW

The work will involve the development of multifunctional photocatalytic films combining Zn–Al layered double hydroxides (LDH) with metal oxides (TiO_2, ZnO, CuO) for dual applications: (1) reduction of volatile organic compounds (VOCs; formaldehyde, toluene) and (2) removal of pharmaceutical pollutants in water (naproxen, diclofenac, ibuprofen, sulfamethoxazole) under UV and later sunlight. This combined platform exploits the fact that LDHs boast exceptional adsorption of pollutants, while LDHs also exhibit good photocatalytic activity, which, in combination with oxides, allows the materials to be tailored for specific applications.

MATERIAL DESIGN JUSTIFICATION

Carbonate-LDH provides a high specific surface area rich in hydroxyls for strong adsorption of pollutants, which is ideal for VOCs or pharmaceutical active ingredients. Chloride-LDH, on the other hand, exhibits high photocatalytic activity (possibly via oxygen vacancies or reactive chlorine species). The incorporation of CuO, which absorbs visible light (e.g., ~1.2–1.7 eV) together with TiO_2 or ZnO, creates p-n heterojunctions with cascade charge

transfer, which broadens the spectral response across the blue-red wavelength range while suppressing recombination.

VOC REDUCTION (GAS PHASE APPLICATION)

Contaminants at ppb–ppm concentrations in indoor air require strong adsorption onto a high-surface-area layer, followed by photocatalytic mineralization into CO_2 and H_2O. LDH-oxide composites provide dual functionality: Si–OH and Al–OH sites adsorb polar VOCs (e.g., formaldehyde) via H-bonding and aromatic compounds (e.g., benzene, toluene) via π-π stacking, while oxide nanoparticles photooxidize the adsorbed substances under light. The p-n heterojunction spatially separates charge carriers, thereby extending lifetime and quantum efficiency. Porous layers (2–50 µm) maximize catalyst adsorption, while hierarchical porosity (micropores for surface area, mesopores for transport, macropores for gas flow) ensures access of pollutants throughout the entire depth of the film.

REMOVAL OF PHARMACEUTICAL ACTIVE INGREDIENTS (USE IN THE AQUEOUS PHASE)

Pharmaceutical micropollutants at concentrations of ng/L–µg/L require preconcentration via adsorption onto photocatalytic layers in flow-through reactors. Adsorption, which depends on speciation (anionic pharmaceuticals are adsorbed at pH 5–7 onto positively charged LDH surfaces via electrostatics and π-π interactions), causes the contaminant to concentrate near photocatalytically active sites. Irradiation with appropriate energy generates e^-/h^+ pairs; holes oxidize pharmaceuticals or generate ·OH, while electrons reduce O_2 to $\cdot O_2^-$. Complete mineralization to CO_2 (confirmed by TOC analysis and absence of toxic intermediates via LC-MS) prevents the accumulation of undesirable products. The inclusion of TiO_2 enables additional UV absorption and strongly oxidizing holes (+3.1 V compared to NHE) that can attack stable aromatic rings. Advanced material configurations, e.g., the combination of carbonate-LDH-CuO (adsorption) with chloride-LDH-CuO (rapid photocatalysis), optimize overall removal efficiency.

FILM PRODUCTION

The films are prepared using various techniques: doctor-blade, dip-coating, spray-coating, and then heat-treated at 200–400 °C to decompose LDH into mixed metal oxides, while maintaining hierarchical porosity due to the evolution of carbonates/chlorides. Glass, metal, or ceramic substrates allow for different thermal loads and options for installing different reactors.

MECHANISTIC STUDIES AND OPTIMIZATION

The alignment of bands at LDH-oxide heterojunctions (type II versus Z-scheme) will be clarified by advanced photoluminescence measurements, photometrics, and electrochemical impedance spectroscopy to optimize charge separation. Radical scavenging experiments (tert-butanol for ·OH, benzoquinone for $\cdot O_2^-$, EDTA for h^+) will identify the dominant reactive oxygen species. Quantification of intermediates via LC-MS will reveal the most suitable materials with the best environmental impact via end products (complete oxidation to CO_2 and H_2O, monitored by TOC analysis).

IMPACT

The successful development of such coatings can later be applied in: (1) HVAC integration for continuous indoor air purification, (2) facade coatings for outdoor VOC reduction, (3) flow-through water purification reactors for removing pharmaceutical contaminants in decentralized systems.

KEY INNOVATIONS:

(i) Dual functionality with LDH carbonate versus chloride selection; (ii) visible light activity through CuO integration and p-n heterojunctions; (iii) Hierarchical porosity that maintains a high surface area in thick layers; (iv) Scalable coating methods compatible with industrial production; (v) Unified platform for solving air and water pollution with a common photocatalytic mechanism.

5. Priloge, ki jih je treba priložiti ob prijavi *(Documents required to be submitted with the application)*:

☒ **potrdilo o doseženi izobrazbi *(proof of completed education)***

- kandidat z zaključenim magistrskim študijskim programom (2. bolonjska stopnja)
  (candidate who has completed a Master's degree (2nd Bologna level)):

  - diplomska listina / potrdilo o zaključku študijskega programa
    (diploma certificate / certificate of completion of the study programme)

  - priloga k diplomi / potrdilo o opravljenih obveznostih
    (diploma supplement / official transcript of records containing all grades obtained in the study programme)

- kandidat, ki še ni zaključil študija na 2. stopnji
  (candidate who has not yet completed a Master's degree):

  - potrdilo o do sedaj opravljenih obveznostih z ocenami magistrskega študijskega programa, s katerim se bo kandidat prijavil na doktorski študij
    (official transcript of records listing all courses and grades obtained so far in the Master's degree programme on the basis of which the candidate will apply for enrollment in a doctoral degree programme.)

☐ **nagrade –** univerzitetna Prešernova nagrada ali Prešernova nagrada članice Univerze v Ljubljani oz. druga enakovredna nagrada *(awards, e.g. Prešeren Prize of the University of Ljubljana, Prešeren Prize of a University of Ljubljana member and/or another equivalent award))*

☒ **bibliografija** *(bibliography)*

☒ **življenjepis** *(CV)*

☒ **motivacijsko pismo** *(motivation letter)*

☒ **opis dosedanjega sodelovanja pri raziskovalnem delu** *(description of the candidate's research work)*

☐ **osnutek idejne zasnove raziskovalnega dela** *(preliminary research proposal)*

☐ **priporočilno pismo** *(letter of recommendation)*

☐ **druge priloge** *(other attachments):*