REVIEW

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Current stage and future development of Belgrade collisional and radiative databases/datasets of importance for molecular dynamics

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Atomic and molecular (A&M) databases that contain information about species, their identities and radiative/collisional processes are essential and helpful tools that are utilized in many fields of physics, chemistry, and chem/phys-informatics. Errors or inconsistencies in the datasets are a serious issue since they can lead to inaccurate predictions and generate problems with the modeling. This demonstrates that data curation efforts around A&M databases are still indispensable and that in the curation process studious attention is required. Therefore, we herein present research activities around Belgrade "nodes" – datasets of collision/radiative cross-sections and rates needed for spectroscopy analysis in various A&M, optical and plasma physics fields. Methodologies of our research and both present and future aspects of the applications are explained. We explored the possibility to extend our nodes towards building a new database on Judd–Ofelt parameters by using machine learning in order to predict optical properties of luminescence materials. In addition, we hope that public availability of our datasets and their graphical representations will also motivate others to investigate the potential of these data.

1. Introduction

Atomic and molecular physics has made huge contributions to our fundamental understanding of nature. The last few decades have seen remarkable progress in both theoretical/computational and experimental techniques applied to the study of radiative and collisional processes involving atoms and molecules.[1,2] Such research has required coordinated studies to provide benchmark data which not only contribute to fundamental science but also have practical implications in various applications and play a crucial role in various fields of science and technology, including astrophysics and space science, plasma physics, nuclear physics, materials science, semiconductor industry, atmospheric sciences, the chemistry of the interstellar medium, medicine, radiation damage and therapy *etc.*[3–8]

Amongst the most important atomic and molecular processes are those involving collisions. Collisional processes involve interactions between particles, such as atoms, molecules, ions, electrons, photons, resulting in energy transfer, scattering, or recombination. These processes are essential for understanding many diverse phenomena including gas dynamics, plasma physics, energy transfer and chemical reactions.[9] Electron scattering from atoms and molecules is one of the most important collisional process and has been intensively studied over a long period of time. As a target in the collision process, the theoretical representation of molecules acquires a new point of view from the mathematical perspectives of energy quantification methods.[10–12] Electron impact collision cross section databases over a wide range of impact energies are required to model and underpin the interactions in various applied fields[13] while total cross section data are useful for the study of electron transport properties in gases.[14,15] The last few decades have seen tremendous progress in both the computational and experimental techniques applied to study the scattering of electrons by biologically relevant molecules. Much ongoing effort has been undertaken to provide a deeper insight into the mechanisms related to the radiation damage of DNA, which includes many processes (ionization, electronic, rotational, and vibrational excitations, dissociation and dissociative electron attachment). Recently, Ebel and Bald[16] presented the first absolute quantification of the energy-dependent strand breakage of a specific sequence of double-stranded DNA by the low-energy electrons

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(LEE) in the energy range of 5–20 eV (providing accurate quantification of DNA radiation damage of well-defined DNA target sequences in terms of absolute cross sections for LEE-induced DNA strand breaks). An overview of the various applications of collision physics with an emphasis on the importance and power of theoretical and computational techniques has been recently provided by Srivastava and Fursa.[17] Recent progress in obtaining experimental benchmark data and the development of highly sophisticated computational methods for use in plasma-using technologies is highlighted in the papers Bartschat and Kushner[18] and Schippers et al.[19]

Particle transport and energy deposition are also one of the essential aspects of processes driving physics and chemistry in the local environment of the collision event. Such processes involve the movement of particles, such as atoms, molecules, or subatomic particles, and the transfer of energy to the surrounding medium. Ongoing research on particle transport and energy deposition aims to improve our knowledge of these processes, leading to advances in areas such as fusion energy (the transport of charged particles is fundamental to understanding phenomena like plasma confinement and fusion reactions), nuclear physics (the deposition of energy by high-energy particles can lead to nuclear reactions or the creation of ionizing radiation), and local chemistry (energy deposition plays a crucial role in processes like chemical reactions, where energy is transferred between reacting species, leading to the breaking or formation of chemical bonds).[20–22]

Radiative processes involve the emission, absorption, and scattering of electromagnetic radiation by atoms, molecules, and particles.[23] They are crucial for investigating the behavior of light and its interactions with matter, as well as the study of various astrophysical phenomena, including stellar spectra, interstellar medium, and cosmology.[24] Spectroscopic techniques provide valuable information about the composition and properties of materials and celestial objects. Ongoing advancements in spectroscopy, including high-resolution and multi-wavelength observations, enable scientists to study distant galaxies, planet atmospheres, and diagnose various materials.[25–29] Study of radiative processes help us to understand how radiation propagates through different media, such as planetary atmospheres, interstellar clouds, and biological tissues[30] Radiative processes also play a crucial role in quantum optics and quantum information science. Controlling and manipulating the emission and absorption of individual photons is crucial in developing quantum cryptography, quantum computing, and quantum sensing.[31]

As one can see, atomic and molecular (A&M) databases are indispensable tools that support scientific research, technological advancements and innovation in a wide range of disciplines (Fig. 1). They can help solve open questions and challenges on the interaction dynamics of molecules and clusters in the gas phase like "How do molecules form and survive in the interstellar medium?" "What are the conditions and the mechanisms?", etc. (see e.g. Gatchell & Zettergren[32]). Here we present research activities in Belgrade that develop databases on collision/radiative cross-sections, describe the development and some technical aspects of the databases, summarize some recent and future developments and currently planned updates and outline our plans for the near future.

The BG A&M databases status, challenges and directions are presented in Section 2, while the technical aspects are presented and discussed in Section 3. Section 4 describes building the rare earth data base supported by machine learning (ML) approach. Finally, Section 5 is devoted to some conclusions.

2. Belgrade nodes: status, challenges and directions

A Virtual Atomic and Molecular Data Center (VAMDC) "node" is a separate software entity implemented by a data provider,
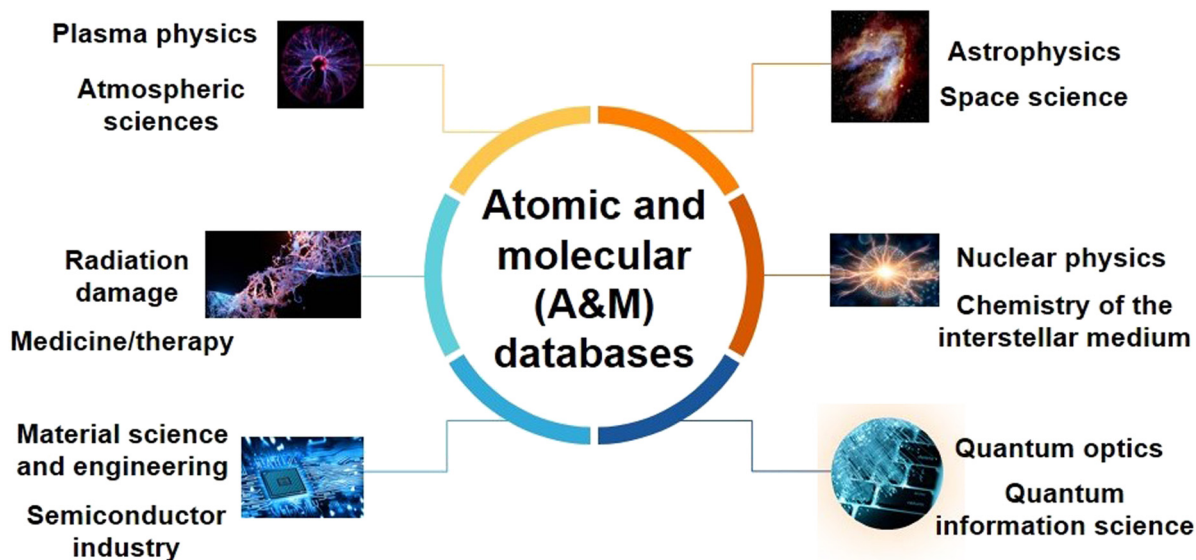

Fig. 1 A&M data and databases play an important role in various fields of science.

which consists of a database and web services compliant to VAMDC standards and protocols.[34] In practice, this is most often implemented using VAMDC-developed NodeSoftware and adapting it for specifics of the particular dataset and technical environment, on top of which custom web interface and additional (graphical) tools may be built.

Atomic and molecular databases and data are becoming increasingly important for data interpretation, diagnostics, and the development of models and simulations of complex physical processes.[35–39] The Belgrade radiative and collisional nodes of VAMDC are hosted by the Serbian Virtual Observatory (SerVO) and currently consists of three databases BEAMDB (**https://servo.aob.rs/emol**) and MolD (**https://servo.aob.rs/mold**) and ACol (**https://servo.aob.rs/acol**). These databases are complementary with other available databases covering similar collisional processes, like KIDA[36] and LXCat databases.[40] While KIDA is more oriented towards astrochemistry and LXCat towards processes in plasmas, our databases cover data of astrophysical relevance. However, the data and its analysis highlight their interdisciplinary nature and usage, *e.g.*, in physics, astrophysics, chemistry and biology.

2.1 BEAMDB-Belgrade electron-atom(molecule) database

The early stages of Belgrade database development started in 2007 with the creation of the Information system in atomic collision physics.[41] In this paper some fundamental aspects of scientific research in the field of atomic physics were discussed where the information system was designed to cover several phases of research from planning the scientific study and literature survey to the creation of databases and dissemination of the results. In conformity with the objectives of two COST (Co-operation in Science and Technology) Actions, P9 Radiation Damage in Biomolecular Systems (RADAM-**https://www.cost.eu/actions/P9/**) and MP1002 Nano-scale insights in ion beam cancer therapy (Nano-IBCT-**https://www.cost.eu/actions/MP1002/**), we developed a particular database[42] in which data from electron interactions with atomic and molecular targets are maintained with the focus on electron-metal atom cross-sections. In the broad scope of the RADAM database[43] that covers processes from elementary ones to multi-scale and biological effect processes, BEAMDB represents a node that is restricted to processes governed by electron impact. When RADAM database was invited to join the VAMDC project[34] BEAMDB became part of that network.[44]

Once BEAMDB had been established attention was turned towards the exploitation of data maintained within it. The first successful usage was in the study of electron scattering cross sections, data needs and coverage in BEAMDB Database for the Rosetta Mission[46] where the direct evidence for the role of electron induced processing was plainly visible. The emission lines observed in the coma of Comet 67P/Churyumov-Gerasimenko during the Rosetta mission were able to be shown to be due to electron rather than photo induced dissociative excitation. The turbulent processes in solar wind on its routes emerging from the solar corona have been remotely measured[47] revealing the existence of two classes of electrons, "warm" and "suprathermal", while the interaction of the solar wind and the comet have been analysed as a function of

heliocentric distance.[48] These observations led to the development of a fully 3D kinetic model which simulates the ion and electron dynamics of the solar wind interaction with a weakly outgassing comet 67P covering the complete energy distribution of electrons.[49] The model draws on data in the BEAMDB.

The BEAMDB database has also been used in a survey of existing cross section data for elastic electron scattering by methane in order to compare present measurements at the Institute of Physics Belgrade (IPB)[50] with those available in literature. The strength of interactions of electrons with a methane molecule is characterised by cross-sections which need to be accurately determined using both experiment and theory. A combined experimental (electron spectrometry measurements) and a theoretical (using two approximations: a simple sum of individual atomic cross-sections and the other with molecular effects taken into the account) study had been performed where differential, integral and momentum transfer cross-sections in the intermediate energy range (50–300 eV) have been obtained.[50] Absolute values of elastic cross sections were obtained by using relative flow method[51] in comparison with known cross sections of argon as a reference gas.[52] In the experiment, effusive beam properties had been predicted and optimized following the work of Lucas.[53]

Regarding data on electron scattering from metal atom vapours, many of the most important cross sections have been assembled at the IPB using a specifically designed electron spectrometer for handling the metal vapours.[55,56] The procedure of obtaining the absolute cross sections for electron scattering by metal atom vapours is different than for other gases. Here the relative flow method can not be performed and we need to rely on other normalisation methods such as converting relative differential cross sections (DCSs) to generalised oscillator strength curves and extrapolation of these to the well-known optical oscillator strength in the zero squared momentum transfer limit.[57] Lassettre formula may then be applied in order to put cross sections an absolute scale using the DCSs for the $6^1 P_1$ state of mercury[58] as reference. An additional improvement has been achieved with the development of forward scattering function method.[59] This method has been applied for electronic excitations of resonant lines of zinc,[60] lead[61] and most recently cadmium.[62]

Molecular dynamics induced by electron impact has been extensively studied. As an example of the low energy dissociative electron attachment process we refer on the case studies of ozone[63,64] where resonant collisions induce formation of atomic and molecular oxygen anions with large cross sections having important consequences for the anion formation processes in the ionosphere. The shape resonances were observed in vibrationally inelastic differential cross sections with long progressions and numerous combination vibrations for all three vibrational modes in energy loss spectra of ozone.[64] In BEAMDB we stored data for DCS for vibrational excitation from the ground state $v = 0$ to the $v = 1$ of furan molecule calculated on the basis of the unitarized first Born approximation (UFBA) by Čurik.[33] Here all 21 modes[65] were summed and presented in Fig. 2.

Another example of the importance of electron collisional processes in molecular dynamic studies is presented in the
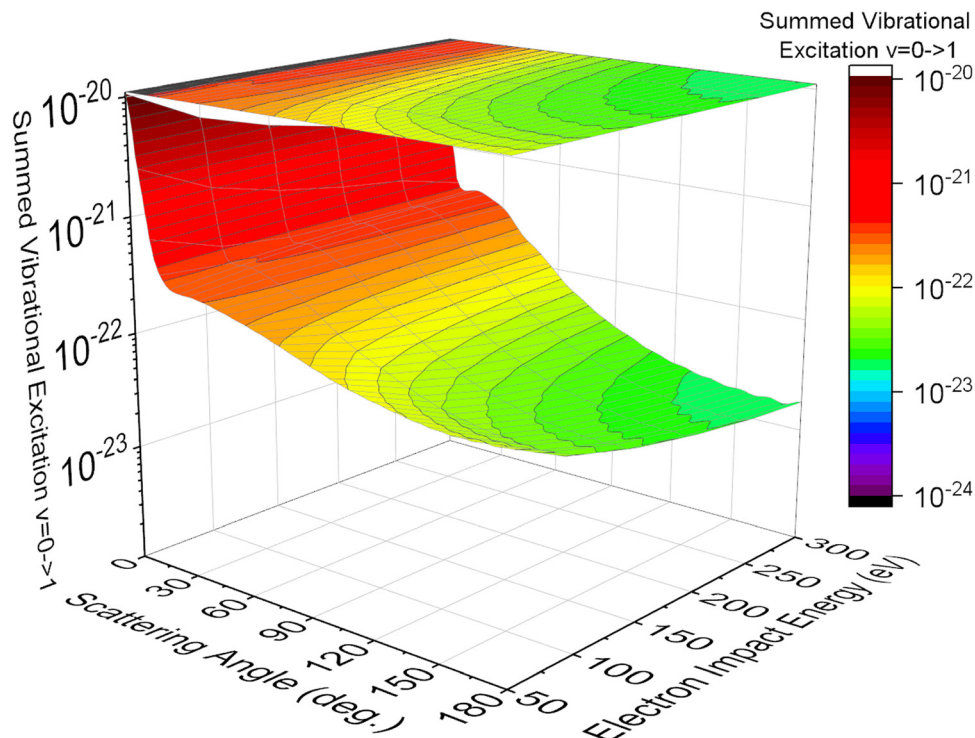
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Fig. 2 Sum of 21 modes for rotationally summed 0 → 1 vibrationally inelastic absolute differential cross sections for scattering of electrons by furan molecule, calculated by UFBA method. The dataset is presented in Maljković *et al.*[33]

simulations of focused electron beam induced deposition (FEBID). Upon the irradiation of metal containing precursor molecules by high energy electrons the molecule is dissociated resulting in deposition of the metal on the irradiated surface. The process is governed by the convolution of flux densities of primary electron beam, secondary electrons and back scattered electrons and the fragmentation cross section of the precursor molecule.[66] Dissociative electron attachment (at electron energies below the first ionization energy), dissociative ionization (at higher electron energies) and neutral dissociation are the processes responsible for the fragmentation of precursor molecules. One of the applications of the FEBID process is presented in nanofabrication of $Pt/TiO_2/Pt$ memristor device[67] obtained from electron irradiation by trimethyl(methylcyclopentadienyl)platinum(IV) used as a precursor for Pt–C electrode deposition and titanium isopropoxide used as a precursor for the TiO_2 layer.

2.2 Photodissociation—The MolD Database

As part of SerVO and VAMDC MolD is made up of a number of parts, including tools for data collecting and user interfaces (*e.g.* AJAX-enabled queries and visualizations on-site). The MolD database includes information on several molecular species their excited states characterizations and photodissociation cross sections in different rovibrational states. These cross sections can be used to obtain average thermal cross sections (see Fig. 3), rate coefficients for non-local thermal equilibrium models and feed into models of various atmospheres, laboratory plasmas and are used in several technological applications.[68–73]

The MolD database was developed in several stages. The first one, which was finished at the end of 2014, was distinguished by the development of a web interface, certain utility programs, and a service for all photodissociation data for hydrogen and helium molecular ions.[74] In each subsequent stage, the web service and utility programs (that allow online data visualization of a wide range of data were developed) were upgraded and new species (MgH^+, HeH^+, LiH^+, NaH^+, H_2^+, He_2^+ …) with photodissociation data are added.

The cross section datasets are obtained using a quantum mechanical method in which the photodissociation process is represented as the result of radiative transitions between the ground and the first excited adiabatic electronic state of the molecular ion (see *e.g.* Sreckovic *et al.*[75] and references therein). In the dipole approximation, the transitions result from the interaction of the electronic component of the ion-atom system with the electromagnetic field.[76]

On-site assistance† is available from MolD, which also provides average thermal cross sections based on the temperature for a particular molecule and wavelength. Plotting of average thermal cross-sections along with available wavelengths for a given temperature is made possible by additional on-site utilities in addition to operating as a VAMDC compatible web service, accessible through the VAMDC portal, and other tools created using VAMDC standards.

As part of SerVO and VAMDC, MolD is heavily utilized by astrophysicists to model stellar atmospheres,[77–79] *etc.* However,
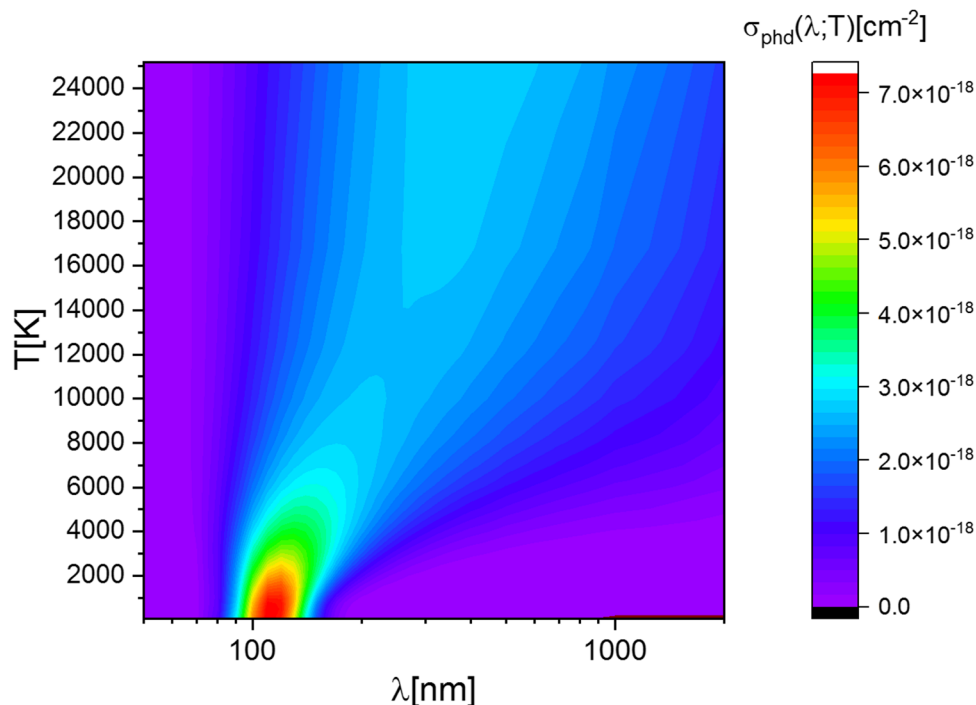
† https://servo.aob.rs/mold/

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Fig. 3 The surface plot of average cross-section for photodissociation, against λ and T, of H_2^+ molecular ion. The dataset is obtained in Srećković *et al.*[45]
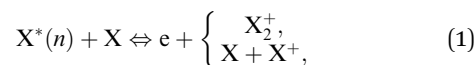
the data can be used for a variety of purposes, including plasma chemistry or experiments like the PLEIADES synchrotron,[80–82] as well as plasma fusion, industry, and for several technology applications.[83–85]

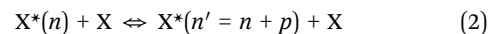### 2.3 ACol-database for collisional processes

Moving from the cold gas approximation to the state-to-state approach, the A&M community has demonstrated a growing maturity in developing processes for curating dynamical data pertinent to the kinetic modeling of low temperature plasmas (LTPs), with the goal of furthering the understanding of fundamental processes involving both electron and heavy species collisions.[86–94] It has recently been shown that research in the food industry and technology suggest the potential usage of plasmas in the treatment of plants such that they may be treated without pesticides or other toxic agents.[95,96] Accordingly A&M datasets of interest for the bio/chemistry and food industry, which include electrons and ions collisions with small molecules and various excited species, are being made available.[97]

As noted ACol comprises the rate coefficients for the collisional processes of excitation/deexcitation and ionization/recombination in hydrogen, helium, and alkali plasmas. The ACol database is now in development. The dataset may be useful for studying and simulating LTP in the lab as well as weakly ionized layers in various atmospheres, *etc.* Moreover the existence and development of the ACol database/node might be crucial for diagnostics and modeling of LTPs which are used for the bio/chemistry and food industry.[98–100] The ACol database is composed of collisional data for excitation/deexcitation and ionization/recombination processes.

The database is made up of collisional ionization/recombination

$$X^*(n) + X \Leftrightarrow e + \left\{ \begin{array}{l} X_2^+, \\ X + X^+, \end{array} \right. \quad (1)$$

and excitation/deexcitation

$$X^*(n) + X \Leftrightarrow X^*(n' = n + p) + X \quad (2)$$

data obtained at the IPB. Here X, X^+ are atoms and their ions in the ground states, $X^*(n)$ are the Rydberg atoms (RA), and X_2^+ their molecular ions. The above mentioned processes are such that system goes through the phase where its parts can be described as a collisional quasi-molecular ion-atom complex.

Fig. 4 presents rate coefficients for associative ionization (upper) and non-associative ionization channels (lower) of eqn (1) as a function of n and T for X = H.

ACol presents cross-sections and rate coefficients for the ionization/recombination and excitation/deexcitation processes for hydrogen, helium and alkali plasmas, for conditions of interest in the laboratory, in astrochemistry and in LTPs. The results were acquired within the DRM, which means that the collisional reactions were handled by the so-called dipole resonant mechanism (DRM) (see Mihajlov *et al.*[101] and references therein). The processes in this characterisation are driven by the dipole component of the electrostatic interaction between the outer highly excited ion-atom system and the inner (ion-atom) system. This technique works especially well when used with the so-called decay approximation. The details can be found in a set of papers.[101–103]

The ACol database is hosted by SerVO **https://servo.aob.rs/acol/**. The queries are hosted locally on the website which also
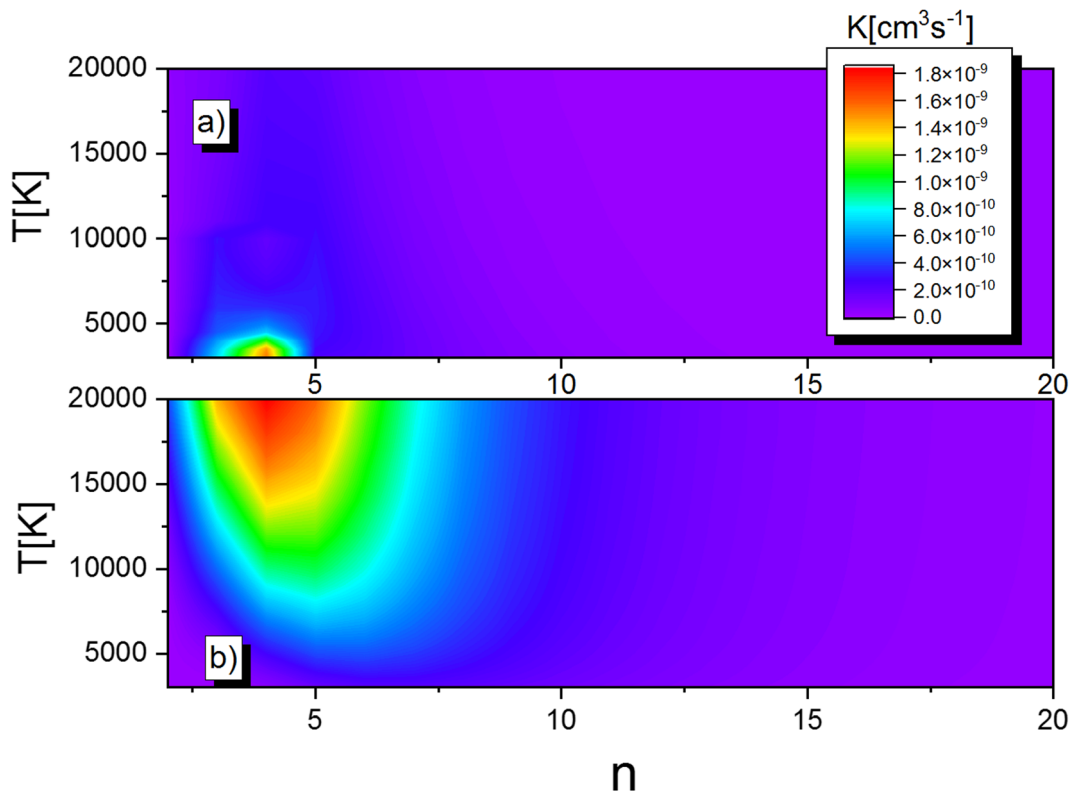
Fig. 4 (a) Rate coefficient for associative ionization channel (upper) of eqn (1) as a function of n and T for the case X = H. (b) same as a) but for non-associative ionization channel (lower) of eqn (1). Dataset is obtained in Srećković *et al.*[54]

deliver data in XSAMS format defined by VAMDC[36] (**https://servo.aob.rs/acol/**) *via* AJAX-enabled web page. On-site, we included an additional collisional processes dialogue box for the XSAMS query and added visual representations of temperature depending cross sections for the new datasets. Web service requests are handled by Python-based NodeSoftware which works on top of a relational database and is available for queries *via* a centralized portal (**https://portal.vamdc.eu/vamdc_portal/home.seam**).

3 Technical aspects of databases and web services

From their initial stages of development, the Belgrade A&M databases have been closely connected with the Virtual Atomic and Molecular Data Center project (VAMDC-**https://vamdc.eu**). In the technical sense, we adapted our data models so they can easily convert to the VAMDC tree-structured serialization schema XSAMS.[104] For BEAMDB-the database which was implemented first-we specialized a data model suited for collisional reactions, with A&M data presented with two X axes for energy and angle and one Y axis for differential cross sections. Next we implemented a photodissociation database with (radiative) processes and somewhat simplified data model which fit the needs of the MolD dataset. For the third node-ACol-with the collisional data, we took the BEAMDB data model as a base, with major revisions such as insertion of polymorphic behaviour into

species and species states, which are inherited by atoms/molecules and atomic states/molecular states, respectively (shown in Fig. 5). This way, flexibility and independence is achieved regardless of type of species which participate in the process. All databases are stored on a MariaDB server (an open-source relational RDBMS system based on MySQL) with regular backups.

In a recent paper,[105] the VAMDC e-infrastructure was evaluated using FAIR methodology[106] made by Research Data Alliance. Using guidelines ratified half decade after the NodeSoftware was implemented, VAMDC scored satisfactory except for licence policy (this is more of a legal issue which gets complex because the international nature of the project) and provenance. As stated in the paper, the provenance shortcoming is based on the lack of implementation of an accepted community standard which would ease automation. This flaw might be critical in scenarios with data workflows, but these kind of orchestration tools aren't yet being developed.

4 Future development

4.1 Building the rare earth data base supported on the Judd–Ofelt theory using machine learning approach

The Judd–Ofelt (JO) theory[107–111] is a remarkably significant theoretical scientific contribution with vast applications in chemistry, material science, and their various academic progenies. Such applications include solid-state lasers, thermal sensors, optical amplifiers, up-conversion, and various biological contexts.[112] One

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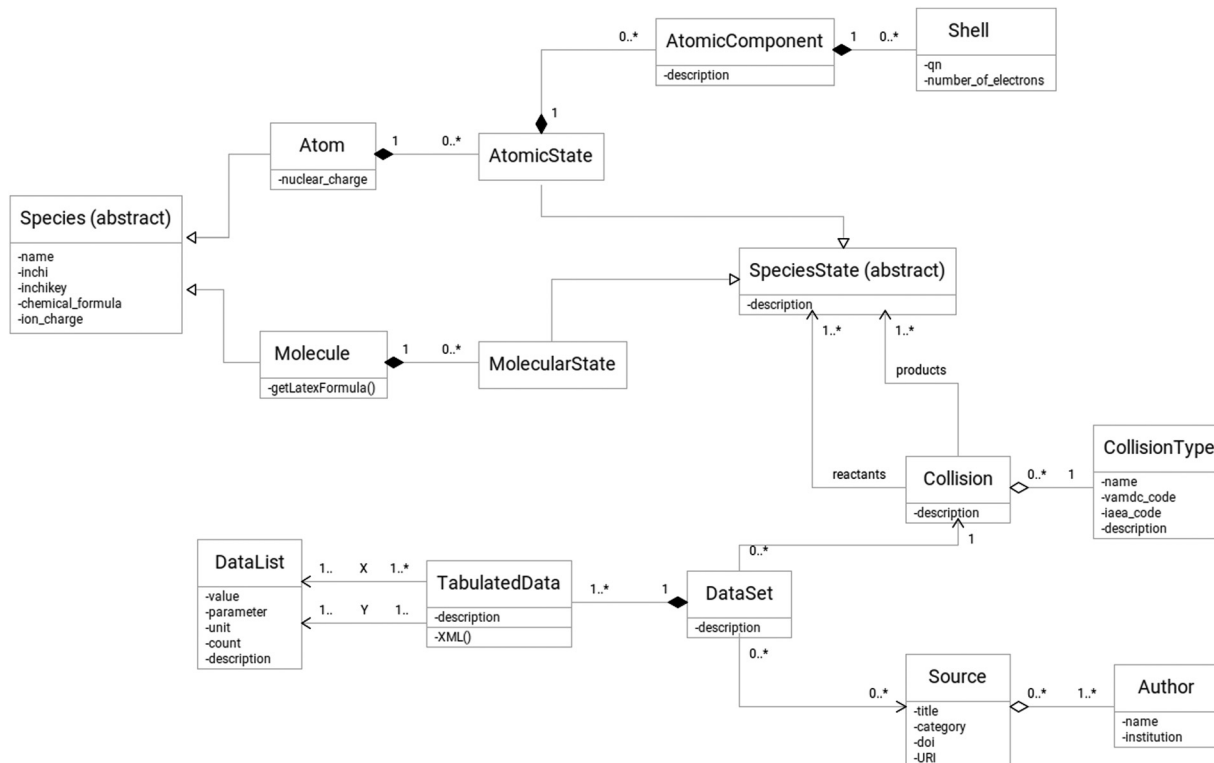*Phys. Chem. Chem. Phys.*, 2023, **25**, 26972–26985 | **26977**

Fig. 5 UML class diagram for the ACol node (logical model).

of the main uses of JO theory in these, and indeed many other applications, is to provide a characterization of a materials optical properties. Moreover, use of JO parameters is a convenient tool for predicting materials characteristics,[113–117] and we have decided to build our own database with JO parameters (henceforth described as JO Database). JO parameters can be calculated from experimentally obtained emission and excitation spectra of Rare earth doped materials.[114–120] A Typical time-resolved spectrum of rare earth doped phosphor (YVO_4:Eu) acquired in our measurements is shown in Fig. 6. Europium transitions are denoted, the insert shows CIE plot (color coordinate diagram) calculated from spectral data.

There are several software applications for calculation of JO parameters, devoted to some specific cases, for example when europium is used as dopant. We will develop our software to be able to add data to JO Database for those materials which have optical spectra available in literature. Once the JO parameters are known for a specific phosphor important optical properties can be calculated. The rate of spontaneous radiative decay for an induced electric dipole (ED) and the magnetic dipole (MD) optical transitions and the resulting radiative lifetime are easy to calculate.[109,111] The total lifetime can be measured experimentally and the non-radiative lifetime and quantum efficiency for emission can be determined.[121]

4.1.1 Machine learning approach. Use of ML to predict optical properties of materials is still a novel approach but one that has already shown significant success and great promise. One of the main advantages it offers is that in principle it removes the need to perform difficult and expensive experiments in order to estimate the spectrum of new rare earth doped inorganic phosphors.

Phosphors with a rigid structure and hence with higher Debye temperature tend to have a low probability of nonradiative relaxation and a favorable quantum efficiency. In recently published works[122,123] ML techniques have been used for predicting Debye temperatures and screening inorganic phosphor hosts. The ML model to predict Debye temperature first required training using a large, diverse set of data,[122,123] obtained from available databases. However, it should be pointed out that material with high quantum yield will not necessarily have color of light useful for artificial lighting of plants or comfortable for human eye, or luminescence lifetimes appropriate for LED display or have characteristics of good thermo-phosphor. Electronic structure descriptor for the discovery of narrow-band red-emitting phosphors are studied in ref. 124 So, our research will not be restricted only to materials with high quantum yield.

ML techniques are also used in another interesting publication where it is described how to predict JO parameters based on the bulk composition in the case of Er^{3+} doped tellurite glasses.[112] The matrix compositions were used to predict the three JO intensity parameters using support vector machine regression, coupled with sparse principal component analysis. This work is very important because it proves that it is possible to predict JO parameters using ML techniques.

In our recent publications[125–127] we have used ML to estimate temperature of thermo-phosphors, plasma electron temperature and laser ablation of printed circuit boards all based on line
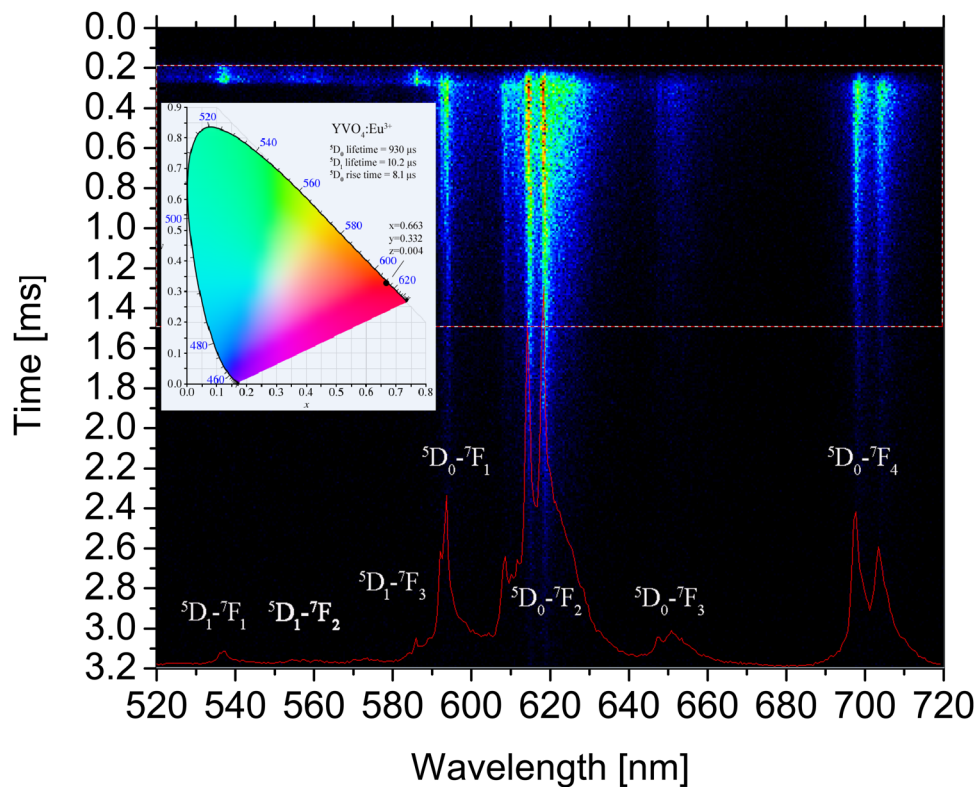
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Fig. 6 Typical time-resolved spectrum of rare earth doped phosphor (YVO₄:Eu) acquired in our measurements. Europium transitions are denoted. Inset shows CIE plot (color coordinate diagram) calculated from spectral data.

profiles in experimentally obtained spectra. So, it seems natural to us to try to connect JO parameters with the spectral shapes of Rare earth doped materials using ML.

We can apply ML techniques to a wide class of known phosphor materials in order to predict their optical properties, improve on the existing results, extend the methods to be used for an arbitrary combination of host and rare earth dopants, build a comprehensive database of optical properties for such materials, and finally provide easy access to these results to interested users. To achieve this, we will first test and select the best performing ML algorithms and train them to predict JO parameters on a suitable subset of materials of well known optical properties, based on a set of material properties available in online materials databases. Trained algorithms can be used to predict optical properties for a wide set of materials available in materials databases for any new host represented by a list of N descriptors. This would in principle allow for an estimation of JO parameters (and hence optical properties) for a large number of as of yet unsynthetized host-dopant combinations. Such a possibility would be of great value to any researcher searching for a material with favorable optical properties, as it would remove the need to go throug a laborious and potentially costly synthesis/experiment procedure. The results obtained can be used to populate a database of JO parameters (with corresponding optical properties) for all already available materials, as well as for a large number of pregenerated host-dopant combinations.

A block diagram of our proposed building and application of JO Database is shown in Fig. 7. Our method consists of several steps. First, we construct a database containing information available directly in the literature and our previous publications.[125,128–137] Where missing the JO parameters will be determined by ML. JO parameters can be used to predict quite practical characteristics of phosphors like luminescence lifetime, CIE color coordinates (color of light as seen by human eye), thermal behavior if used for remote temperature sensing, including useful range of temperature measurements and sensitivity. Other relevant data, like all basic information about structure of the material and the Debye temperature, will be also added to the JO Database. Typical characteristics of phosphors and their importance in applications are summarized in Table 1. Finally, estimates of the JO determined parameters and the optical characteristics of the materials and their possible applications will be added to JO database.

4.1.2 Integration of data into a new VAMDC node. Web access to the database will be developed, featuring a user interface which will allow users to easily find any available host-dopant combination with desired optical properties (whether imported from existing material databases or one of the generated combinations). When queried for materials with certain characteristics, or combinations of characteristics, the JO Database is expected to show which material has the closest characteristics to those desired by the user. In addition, an extended functionality would allow the users to submit their
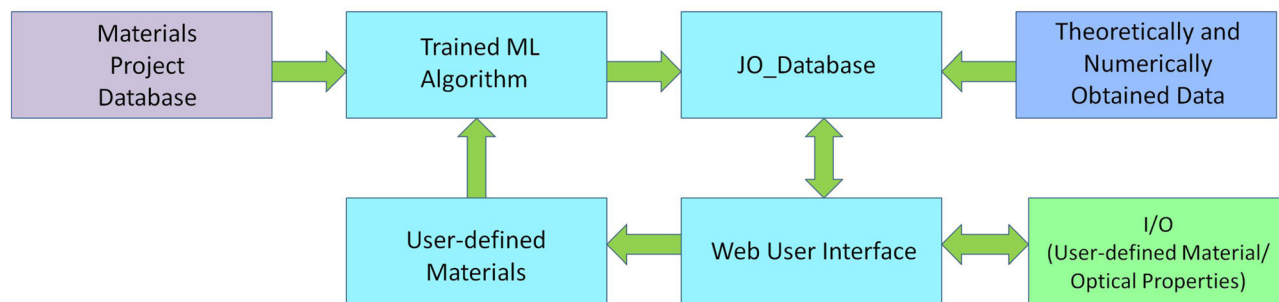
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Fig. 7 Building and application of JO database.

own combination of a host crystal and rare-earth dopant, if it is not already included in the database.

The development of the VAMDC node for the rare earth dataset will begin with writing a data model which fits into the XSAMS tree structure. The excitation and emission spectra will be presented *via* Radiative process, *i.e.* radiative transition model, with intensities on Y axis and wavelength and time on two X (or X and Z) axes. In this transition, species (host and dopant) will have their own states which will vary on different parameters, such as excitation wavelength or concentration of dopant element.

4.2 Extension of existing BG VAMDC nodes

Besides the basic principles that govern the maintenance and curation of databases, it is always necessary to follow the current achievements in rapidly growing and innovative IT industry. Also, a paradigm of how the research itself has been conducting is constantly changing in order to provide the answers to the main societal challenges. An open science becomes a golden standard especially when the FAIR data principles (findability, accessibility, interoperability, and reusability) have been introduced.[138] We share the vision of the VAMDC Consortia to provide atomic and molecular data to all researchers and stockholders *via* distributed databases and with a single data portal as an entry point. In that sense database upgrades and new standards include:

• Insertion of newly calculated/measured datasets; It is a constant concern of all data curators to add new datasets within databases. It is not an easy task since data need first to be evaluated (the policy is that all data must be already published and thence peer reviewed), then to add them manually and finally to check for any errors that might arise during the whole process. As this is a very slow process, it needs to be improved by automatic harvesting from other repositories. It is clearly a task that need a distinct project since data are presented with

different standards and all of them has to be converted to VAMDC ones.

• Regular updating of Node Software *i.e.* Python software, Django (**https://www.djangoproject.com/**), *etc.* This may necessitate some adjustments to the customization of each node since upgrades are often not compatible in all APIs.

• ML & DB; Our aim is to provide available machine-readable metadata that would deliver information to interpret data in areas which are our main target of interest, such astrophysics, molecular science, radiation damage of biological targets on the molecular level, environmental science, plasma processes or lighting industry. These machine-readable metadata need to be organised according to machine-actionable reporting guidelines and models.[139]

• Website user interface and on-site new AJAX enabled queries and visualizations/extension; The current version of BEAMDB offers download of data only in xsams format that is not convenient to many users. So, some extension is needed that would transform datasets into usual txt or svc formats. It would also be very convenient to have a graphical representation of 3D data that are covered in the BEAMDB, yuch as differential cross sections for electron elastic scattering or electronic excitations.

5 Conclusions and perspectives

The lack of trustworthy chemical data is one of the difficult issues when modeling plasmas. The BG nodes were created for this reason. This review has summarized the current stage of development of Belgrade nodes of importance for molecular dynamics. The nodes were developed using protocols established by the Virtual Atomic and Molecular Data Centre. The nodes now face the challenge of software upgrades and continuous improvement of data processing due to the rapid expansion of online A&M services required in modern science.

Table 1 Characteristics of phosphors and their importance in applications

Quantum yield	Artificial lighting, light sources, displays
Thermal stability	All applications
Intensity ratio between spectral lines	Remote temperature sensing, color of artificial lighting, light sources, displays
Luminescence lifetime	Remote temperature sensing, displays, bioimaging
Luminescence rise time	Remote temperature sensing, bioimaging

We have explored the possibility of extending our nodes towards building a new database of Judd–Ofelt parameters using ML to predict the optical properties of luminescent materials. These databases are expected to have an impact in many fields of physics, chemistry, and chem/phys-informatics sectors.

Author contributions

All of the authors contributed equally to this work. All authors have read and agreed to the published version of the manuscript.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

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