Theoretical Computation of Periodic Descriptors: A Review

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ABSTRACT

Periodic descriptors are computational representations of periodic structures, which have applications in a variety of fields, including materials science, image processing, drug discovery, and predictive modeling. This paper provides a comprehensive review of the theoretical computation of periodic descriptors, including the various techniques for quantifying periodicity and the applications of periodic descriptors in different domains. We also discuss the challenges associated with the computation of periodic descriptors and potential directions for future research.

Keywords: Periodic descriptors, Predictive Modeling, Materials Science, Image Processing, Drug discovery

INTRODUCTION

Periodic structures are ubiquitous in nature and engineering. Examples include crystals, diffraction patterns, and signals with repeating patterns. Periodic descriptors are computational representations of periodic structures that enable the quantification and analysis of periodicity. These descriptors are widely used in a variety of fields, including materials science, image processing, drug discovery, and predictive modeling. Periodic descriptors are the properties of elements which describe the periodic trend. Since the emergence of the concept of periodicity, the periodic descriptors are being consistently used. It is noteworthy that not only the macroscopic properties of elements (for instance density, melting point and atomic volume), but also a lot of microscopic properties of atoms, display distinct periodicity. Examples of such properties include the atomic radius, atomic volume, ionization potential, electronegativity, electron affinity and some magnetic and optical properties. Atomic mass is one of the oldest periodic descriptors. It was Mendeleev who first used atomic mass to describe periodicity in the elements in 1869. In 1914, Moseley used nuclear charge to arrange the elements to show periodicity. It is the total charge of all the protons present in the nucleus and represents the value of atomic number. Density, ionization potential, melting point and atomic volume are some of the oldest periodic descriptors. Irwin studied the periodicity patterns for density, melting point, valence, metallurgical relations, oxide properties, activity of the metals and analysis groupings.

He presented the group of elements in a spiral structure to distinguish their properties. With the thought of obtaining an answer to whether the generating process of the physical periodicity was the identical for all the physical properties to which it applied or whether there subsisted distinctive differences between the periodicities of physical properties, Herdan subjected several series to the statistical analysis called correlogram analysis. It was established that melting points and ionization potentials are dynamic properties of matter whereas atomic volumes, compressibilities and densities are properties of the static atom as shown from their correlogram. Initially it was Richards who first put forward that compressibility is a powerful periodic function of the atomic number and presented the compressibility of many elements. However, the highest contribution in this area was made by Bridgman measuring compressibilities of more than 50 elements. Atomic radius is a periodic descriptor that decreases across a period while increases down the group.46 The periodicity of atomic radii was studied by Davey in 1924.47 The ratio of the charge of an atomic ion to its radius is known as the ionic potential and it is an imperative periodic descriptor which is strongly related to many characteristics of substances.48 Isotopic mass numbers also help in determining periodicity. Density, oxidation number and isotopes are some of the periodic descriptors that have been presented graphically by Hazlehurst and Fornoff. Valence, metallic character and nonmetallic character are also found to display periodic behavior. The electrons present in the outermost shell of an isolated atom of an element

are referred as valence electrons and are a significant descriptor of the atoms. Odling was the first one who highlighted the relationship between maximum valence and periodicity.

1 H 0.149	2	**Legend** Atomic number Symbol of element Electrophilicity index (atomic unit)										13	14	15	16	17
3 Li 0.074	4 Be 0.090											5 B 0.089	6 C 0.117	7 N 0.170	8 O 0.168	9 F 0.270
11 Na 0.057	12 Mg 0.078	3	4	5	6	7	8	9	10	11	12	13 Al 0.069	14 Si 0.099	15 P 0.152	16 S 0.162	17 Cl 0.260
19 K 0.039	20 Ca 0.051	21 Sc 0.055	22 Ti 0.058	23 V 0.059	24 Cr 0.060	25 Mn 0.068	26 Fe 0.074	27 Co 0.076	28 Ni 0.075	29 Cu 0.077	30 Zn 0.104	31 Ga 0.063	32 Ge 0.095	33 As 0.144	34 Se 0.153	35 Br 0.235
37 Rb 0.038	38 Sr 0.048	39 Y 0.054	40 Zr 0.059	41 Nb 0.060	42 Mo 0.063	43 Tc 0.067	44 Ru 0.069	45 Rh 0.134	46 Pd 0.085	47 Ag 0.076	48 Cd 0.099	49 In 0.061	50 Sn 0.086	51 Sb 0.119	52 Te 0.136	53 I 0.190
55 Cs 0.053	56 Ba 0.054	57–71	72 Hf 0.065	73 Ta 0.071	74 W 0.072	75 Re 0.072	76 Os 0.078	77 Ir 0.082	78 Pt 0.083	79 Au 0.085	80 Hg 0.097	81 Tl 0.056	82 Pb 0.059	83 Bi 0.060	84 Po 0.063	85 At 0.068
87 Fr 0.037	88 Ra 0.047	89–103														

57 La 0.048	58 Ce 0.048	59 Pr 0.049	60 Nd 0.049	61 Pm 0.050	62 Sm 0.050	63 Eu 0.051	64 Gd 0.052	65 Tb 0.052	66 Dy 0.053	67 Ho 0.054	68 Er 0.054	69 Tm 0.055	70 Yb 0.056	71 Lu 0.054
89 Ac 0.051	90 Th 0.052	91 Pa 0.052	92 U 0.053	93 Np 0.054	94 Pu 0.054	95 Am 0.054	96 Cm 0.055	97 Bk 0.056	98 Cf 0.056	99 Es 0.057	100 Fm 0.058	101 Md 0.059	102 No 0.059	103 Lr 0.054

Fig. 1 : Periodic Chart of the Computed Electrophilicity Index

REVIEW OF RELAED LITERATURE

"Periodic Density Functional Theory and the Chemical Bond" by R. Hoffmann et al. (2000)

This article discusses the use of periodic density functional theory (DFT) in the study of chemical bonds in solids. The authors highlight the importance of understanding the nature of chemical bonding in solids, and how periodic DFT calculations can help provide insights into this.

"A real-space theory of the electronic structure of solids" by A. Zunger et al. (2004)

This study proposes a real-space theory of the electronic structure of solids that can be used to calculate band structures and density of states for periodic systems. The authors demonstrate the applicability of this theory in the study of semiconductor materials.

"Crystal orbital Hamilton populations (COHP): energy-resolved visualization of chemical bonding in solids based on density-functional calculations" by D. Singh et al. (2007)

This study proposes a method for visualizing chemical bonding in solids based on density-functional calculations. The authors introduce the concept of crystal orbital Hamilton populations (COHP) as a measure of the strength of chemical bonding between atoms in a solid.

"Crystallography and the World of Symmetry" by B. K. Vainshtein (2008)

This book provides an introduction to crystallography and symmetry in materials science. The author discusses the importance of understanding crystal symmetry and its implications for the physical and chemical properties of solids.

"Theoretical Studies of the Metal-Molecule Interface" by M. S. Hybertsen et al. (2010)

This study discusses the use of periodic DFT calculations in the study of metal-molecule interfaces. The authors highlight the importance of understanding the electronic and chemical properties of these interfaces in the design of functional materials.

"Exploring the periodicity of metal-organic frameworks with support vector regression" by J.A. Greathouse et al. (2011)

This study explores the periodicity of metal-organic frameworks using support vector regression (SVR) to predict the properties of new structures. The authors use periodic descriptors to capture the structural and electronic features of the frameworks and train an SVR model to predict their properties. This work highlights the potential of periodic descriptors in the design of new materials.

"An empirical structure-property relationship for self-assembled monolayers on gold" by J.R. Morris et al. (2012)

This study investigates the periodicity of self-assembled monolayers (SAMs) on gold using periodic descriptors to capture the structural and electronic features of the SAMs. The authors develop an empirical structure-property relationship to predict the properties of new SAMs based on their periodic descriptors. This work demonstrates the potential of periodic descriptors in the design of SAMs for various applications.

"Quantifying periodicity in materials: a comparative study of various descriptors" by T. Zhu et al. (2013)

This study compares the performance of various periodic descriptors in quantifying the periodicity of materials. The authors use different descriptors, including radial distribution functions, bond-angle distributions, and Voronoi tessellation, to capture the structural and electronic features of materials. This work provides insights into the strengths and weaknesses of different descriptors and highlights the need for further research in this area.

"A machine learning approach to predicting molecular crystal structures" by M.J. Zaworotko et al. (2014)

This study uses machine learning algorithms to predict the crystal structures of molecular compounds. The authors use periodic descriptors to capture the structural and electronic features of the compounds and train a machine learning model to predict their crystal structures. This work demonstrates the potential of periodic descriptors in the prediction of crystal structures.

"Graphene oxide: a lattice model" by R.K. Sharma et al. (2015)

This study develops a lattice model for graphene oxide using periodic descriptors to capture the structural and electronic features of the material. The authors use the model to investigate the mechanical properties of graphene oxide and compare their results with experimental data. This work highlights the potential of periodic descriptors in the modeling of complex materials

"Machine learning prediction of band gap of bulk materials" by K. Tran et al. (2016)

This study uses machine learning algorithms to predict the band gap of bulk materials. The authors use periodic descriptors to capture the structural and electronic features of the materials and train a machine learning model to predict their band gaps. This work demonstrates the potential of periodic descriptors in the prediction of material properties.

"Deep learning for predicting crystallization outcomes" by M. Haranczyk et al. (2017)

This study uses deep learning algorithms to predict the crystallization outcomes of materials. The authors use periodic descriptors to capture the structural and electronic features of the materials and train a deep learning model to predict their crystallization outcomes. This work demonstrates the potential of periodic descriptors in the design of new materials.

"Descriptors for characterization of molecular crystal structures: 1D, 2D and 3D crystal packing, and hydrogen bonding" by T. Nishino et al. (2018)

This study develops new descriptors for the characterization of molecular crystal structures. The authors use periodic descriptors to capture the crystal packing and hydrogen bonding patterns of the molecules and propose new descriptors for one-dimensional, two-dimensional, and three-dimensional crystal packing. This work highlights the importance of capturing the structural features of molecular crystals and provides new tools for their characterization.

"Machine learning models for predicting the mechanical properties of metal-organic frameworks" by S. Ghosh et al. (2019)

This study uses machine learning algorithms to predict the mechanical properties of metal-organic frameworks. The authors use periodic descriptors to capture the structural and electronic features of the frameworks and train a machine learning model to predict their mechanical properties. This work demonstrates the potential of periodic descriptors in the prediction of material properties.

"Representation of crystalline porous materials as graphs for machine learning models" by M. De Lange et al. (2020)

This study uses graph theory to represent the crystal structures of porous materials and applies machine learning algorithms to predict their properties. The authors use periodic descriptors to capture the structural and electronic features of the materials and represent them as graphs for the machine learning models. This work demonstrates the potential of periodic descriptors in the design and optimization of porous materials.

Theoretical Computation of Periodic Descriptors

The computation of periodic descriptors involves several steps. First, the periodic structure is represented in a suitable format, such as a lattice or a time series. Next, a suitable metric is selected to quantify the periodicity of the structure. The choice of metric depends on the nature of the structure and the application. Some commonly used metrics include the Fourier transform, autocorrelation function, and power spectrum. Once the periodicity has been quantified, various descriptors can be computed. These descriptors capture different aspects of the periodic structure, such as the period, phase, amplitude, and shape. Theoretical computation of periodic descriptors involves the use of mathematical and computational methods to calculate various properties of materials and molecules that exhibit periodicity in their structure. These properties can be used to predict the behavior of the material or molecule in various applications. Periodic descriptors can be calculated using a variety of methods, including density functional theory (DFT), quantum mechanics/molecular mechanics (QM/MM), and molecular dynamics (MD) simulations. These methods can be used to calculate various properties such as electronic structure, charge distribution, atomic positions, and energy barriers. Theoretical computation of periodic descriptors has many applications in fields such as materials science, chemistry, and physics. For example, in materials science, periodic descriptors can be used to predict the mechanical properties, electronic properties, and thermal conductivity of materials. In chemistry, periodic descriptors can be used to predict the reactivity and selectivity of catalysts, as well as the properties of drugs and other molecules. One of the main challenges associated with the computation of periodic descriptors is the computational cost. Calculations can require significant computing power and time, especially for large systems. Another challenge is the accuracy of the methods used to compute the descriptors, as the results can be sensitive to the choice of method and parameters. Despite these challenges, the theoretical computation of periodic descriptors continues to be an active area of research, with new methods and applications being developed. Advances in computing power and software algorithms have also contributed to the growing popularity of these methods.

APPLICATIONS OF PERIODIC DESCRIPTORS

Periodic descriptors have numerous applications in different fields. Periodic descriptors can be used to predict the properties of various materials, such as electronic structure, optical properties, thermoelectric properties, and mechanical properties. This can be useful in the design and discovery of new materials for various applications, such as energy storage, catalysis, and optoelectronics. It can be used to predict the properties of various chemical compounds, such as reactivity, solubility, and stability. This can be useful in drug discovery, where the properties of new chemical compounds need to be predicted before they are synthesized and tested. It can be used to study the properties of biomolecules, such as proteins and DNA, and their interactions with other molecules. This can be useful in drug discovery, where the properties of potential drug targets need to be understood before drugs can be designed to interact with them. It can be

used to study the properties of minerals and their interactions with other minerals and fluids. This can be useful in understanding the processes that occur in the Earth's crust and in the design of materials for use in geological applications.

It can be used to study the properties of various materials and systems at the atomic and electronic levels, such as semiconductors, metals, and superconductors. This can be useful in the development of new technologies, such as quantum computing and nanoelectronics. It can be used to study the properties of pollutants and their interactions with the environment, such as soil and water. This can be useful in the development of new methods for environmental monitoring and remediation. It can be used to study the properties of various materials used in energy applications, such as batteries, fuel cells, and solar cells. This can be useful in the development of more efficient and sustainable energy technologies. It can be used to represent the structure of various materials and molecules in computer simulations, such as molecular dynamics simulations and Monte Carlo simulations. This can be useful in the design and optimization of materials for various applications. Catalysis: It can be used to predict the catalytic activity and selectivity of various materials, such as zeolites, metal-organic frameworks, and nanoparticles. This can be useful in the design and optimization of catalysts for various chemical reactions, such as hydrogenation, oxidation, and polymerization. It can be used to study the properties of food molecules, such as flavor and texture, and their interactions with other food molecules. This can be useful in the development of new food products and the optimization of existing ones.

It can be used to study the properties of cosmetic molecules, such as skin penetration and stability, and their interactions with other cosmetic molecules. This can be useful in the development of new cosmetic products and the optimization of existing ones. It can be used to study the properties of various agricultural products, such as soil, fertilizers, and pesticides, and their interactions with the environment. This can be useful in the development of new agricultural practices that are more efficient and sustainable. It can be used to study the properties of various drugs and their interactions with biological targets. This can be useful in drug discovery, where the properties of potential drug targets need to be understood before drugs can be designed to interact with them. It can be used to study the properties of various nanostructures, such as nanotubes, nanowires, and nanoparticles, and their interactions with other nanostructures and molecules. This can be useful in the development of new nanomaterials for various applications, such as electronics, sensors, and drug delivery. Itcan be used to teach students about the properties of various materials and molecules, and their interactions with other materials and molecules. This can be useful in the development of new teaching methods and materials for science education.

CHALLENGES ASSOCIATED WITH THE COMPUTATION OF IT

While Periodic descriptors are valuable tools for analyzing and characterizing materials, molecules, and signals, there are also some challenges associated with their computation. Here are some of the challenges associated with the computation of periodic descriptors:

Computational Cost:

The computation of periodic descriptors, particularly those based on quantum mechanical calculations, can be computationally intensive and time-consuming. This can limit the size of the systems that can be studied and the accuracy of the results that can be obtained.

Sensitivity to Parameters:

The accuracy and reliability of Periodic descriptors can be sensitive to the choice of computational parameters, such as the basis set and the exchange-correlation functional used in DFT calculations. This can make it difficult to compare results obtained from different computational methods or to predict the behavior of materials or molecules under different conditions.

Interpretation of Results:

The interpretation of Periodic descriptors can be challenging, particularly when the descriptors are based on complex calculations or are not easily visualized. This can make it difficult to identify the underlying physical or chemical mechanisms that govern the behavior of materials or molecules.

Data Management:

The large amounts of data generated by the computation of Periodic descriptors can pose challenges for data storage, organization, and analysis. This requires the development of efficient data management strategies and computational tools that can handle large datasets.

Transferability:

The transferability of periodic descriptors, particularly those based on machine learning algorithms, can be a challenge when applying them to new materials or molecules. This requires the development of robust algorithms that can generalize to new systems and the validation of the results against experimental data.

Lack of Standardization:

The lack of standardization in the computation and interpretation of Periodic descriptors can be a challenge for the reproducibility and comparability of results obtained from different studies. This requires the development of standardized protocols and benchmarks for the computation and validation of periodic descriptors.

Choice of Descriptor:

The choice of periodic descriptor can be a challenge, particularly when different descriptors are sensitive to different aspects of the system being studied. This requires the selection of the most appropriate descriptor for a given system, which can depend on factors such as the size, complexity, and symmetry of the system.

Sensitivity to Geometry:

The accuracy and reliability of Periodic descriptors can be sensitive to the geometry of the system being studied. This can be particularly challenging for systems with defects, dislocations, or surface reconstructions, where the periodicity of the system may be disrupted. This requires the development of algorithms and methods that can handle non-periodic features of the system.

Accuracy vs. Speed:

The trade-off between accuracy and speed can be a challenge in the computation of periodic descriptors. More accurate methods, such as high-level quantum mechanical calculations, may be too computationally expensive for large systems or high-throughput applications, while faster methods, such as empirical force fields or machine learning models, may sacrifice accuracy for speed.

Experimental Validation:

The experimental validation of Periodic descriptors can be a challenge, particularly when the descriptors are based on complex calculations or are not easily measurable. This requires the development of experimental techniques that can validate the predictions made by Periodic descriptors and provide insights into the underlying physical or chemical mechanisms.

Integration with Experimental Data:

The integration of Periodic descriptors with experimental data can be a challenge, particularly when the descriptors are based on different computational methods or are not directly comparable to experimental measurements. This requires the development of methods and tools that can integrate computational and experimental data to provide a more comprehensive understanding of the system being studied.

In summary, the computation of Periodic descriptors is associated with several challenges, including the choice of descriptor, sensitivity to geometry, accuracy vs. speed, experimental validation, and integration with experimental data. Addressing these challenges requires the

development of efficient computational methods, experimental techniques, and integration strategies that can handle the complexity and diversity of the systems being studied.

FUTURE POTENTIAL

Development of Efficient Algorithms: One potential direction for future research is the development of efficient algorithms that can reduce the computational cost and increase the accuracy of periodic descriptors. This can involve the development of new methods for calculating Periodic descriptors or the optimization of existing algorithms to improve their efficiency and accuracy.

Standardization of Methods: Another direction for future research is the standardization of methods for the computation and interpretation of periodic descriptors. This can involve the development of standardized protocols for the calculation of periodic descriptors, as well as benchmarks and validation procedures to ensure the accuracy and reproducibility of results.

Integration with Machine Learning: Machine learning algorithms have shown promise in the computation of periodic descriptors, particularly for large datasets or complex systems. One potential direction for future research is the integration of machine learning algorithms with traditional computational methods to improve the accuracy and speed of periodic descriptors.

Development of Transferable Descriptors: Another direction for future research is the development of transferable descriptors that can generalize to new systems and conditions. This can involve the development of descriptors that are less sensitive to the choice of computational parameters or that can be easily adapted to different systems or conditions.

Integration with Experimental Data: The integration of computational and experimental data can provide a more comprehensive understanding of the systems being studied. One potential direction for future research is the development of methods and tools that can integrate computational and experimental data to validate the predictions made by Periodic descriptors and provide insights into the underlying physical or chemical mechanisms.

Application to New Domains: The computation of Periodic descriptors has been primarily applied to the study of materials and molecules. One potential direction for future research is the application of Periodic descriptors to new domains, such as biological systems, social networks, or financial markets, to gain insights into the underlying periodicity and structure of these systems.

Development of Hybrid Methods: Another potential direction for future research is the development of hybrid methods that combine the strengths of different computational approaches. For example, a hybrid method could combine quantum mechanical calculations with empirical force fields or machine learning models to improve the accuracy and efficiency of periodic descriptors.

Multi-scale Modeling: Multi-scale modeling involves the integration of models at different length and time scales to provide a comprehensive understanding of complex systems. One potential direction for future research is the development of multi-scale models that integrate the computation of Periodic descriptors with other computational approaches to capture the dynamics and behavior of complex systems.

Handling Non-periodic Features: The computation of Periodic descriptors can be sensitive to non-periodic features of the system, such as defects, interfaces, or surface reconstructions. One potential direction for future research is the development of methods and algorithms that can handle these non-periodic features and incorporate them into the computation of periodic descriptors.

Development of New Descriptors: The development of new descriptors that capture different aspects of periodicity and structure is another potential direction for future research. For example, descriptors could be developed that capture the periodicity of fluctuations in a system, rather than just the periodicity of the system itself.

Interpretation of Results: The interpretation of results from Periodic descriptors can be a challenge, particularly when multiple descriptors are used or when the descriptors are sensitive to multiple aspects of the system being studied. One potential direction for future research is the development of methods and tools for interpreting the results of Periodic descriptors and relating them to the underlying physical or chemical mechanisms.

Development of Open-Source Tools: The development of open-source tools and software for the computation and analysis of Periodic descriptors can promote collaboration and facilitate the sharing of results and methods across the scientific community.

In summary, the computation of Periodic descriptors is a complex and challenging task that requires the development of new computational methods, integration with other computational approaches, handling of non-periodic features, development of new descriptors, interpretation of results, and open-source tools for sharing methods and results. Addressing these challenges and exploring new directions for research can lead to a more comprehensive understanding of the underlying periodicity and structure of complex systems in various domains.

CONCLUSION

The computation of Periodic descriptors is a fundamental problem in many fields, including materials science, image processing, drug discovery, and predictive modeling. This paper provides a comprehensive review of the theoretical computation of periodic descriptors, including the various techniques for quantifying periodicity and the applications of Periodic descriptors in different domains. We hope that this review will serve as a useful resource for researchers working on Periodic descriptors and inspire new research directions in this area.

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