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Editorial

Recent advances in computational materials design: methods, applications, algorithms, and informatics

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Today computation-aided materials design has become an integral part of the materials science research. Directly complementing experimental synthesis and testing, theoretical, computational, and data-enabled approaches have been playing an increasingly important role in both discovery and optimization of novel and improved materials for targeted applications. Over the past decade, the *in silico* materials design ecosystem has largely been fueled by the sustained exponential growth in computational power, algorithmic developments, and wide availability of open-source scientific software [1–3]. More recently, a widespread adoption of artificial intelligence and machine learning-based methods has opened up alternative avenues for materials design and development [4, 5].

This Special Issue is intended to collect some of the most recent developments in this highly active area of computational materials design with contributions highlighting a wide variety of methods ranging from first principles computations to atomistic molecular dynamics methods and from mesoscale methods to machine learning based surrogate model development for materials property predictions. The Special

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Issue begins with a review article followed by topical articles in the areas of "*Atomistic and Mesoscale Methods*", "*Ab-Initio Modeling*", "*Machine Learning*" and culminates with articles that discuss numerical modeling for explaining materials behavior and drug design for SARS-COV-2.

The issue starts with a review article by Christopher Bartel [6] that discusses fundamentals of computing thermodynamic stability of materials using first-principles methods. The stability with respect to decomposition into competing phases as well as with respect to phase transition into alternative structures at fixed composition is discussed with state-of-the-art methods and practical considerations.

This Special Issue highlights topical articles presenting recent advances in atomistic modeling methods that use molecular dynamics simulations. The article by Uberuaga et al. [7] investigates the complex interplay between the alloying elements and the diffusion behavior of atoms and defects at grain boundaries in Ni. The article by Sose et al. [8] investigates the structure and dynamics of confined water in hybrid layered materials. The article by Nikolov et al. [9] demonstrates new capabilities to investigate the interplay between phonon and magnetic spin contributions to the thermal conductivity of α-iron using a new spectral neighbor analysis potential. The article by Mishra et al. [10] demonstrates a new capability to characterize phase and twinning variants in atomistic microstructures using a new virtual texture analysis method. The article by Gupta et al. [11] targets to understand differences in the structural properties of highly charged polyacrylic acid and polymethacrylic acid using atomistic molecular dynamics simulations in the presence of divalent salt magnesium chloride, with a particular emphasis on understanding the differences pertaining to the microstructure, hydrogen bonding, intermolecular structure, and salt-ion distribution around the polymers.

The issue also highlights topical articles presenting recent advances in mesoscale modeling approaches required for computational materials design. The article by Fey et al. [12] extends the phase-field dislocation dynamics method to predict the mobility of edge and screw dislocations in BCC metals. The article by Coutinho et al. [13] demonstrates the capability to use machine learning methods to parameterize phase field models and predict the phase separation behavior in medium entropy alloys. The article by Siddique et al. [14] identifies the capabilities and limitations in modeling the solid solution strengthening behavior using discrete dislocation dynamics method. The article by Izvekov et al. [15] demonstrates a new capability to model shear banding behavior in shocked energetic materials using a coarse-grained modeling method. The contribution by Li et al. [16] utilizes a crystal plasticity finite element model to study fatigue crack initiation in the high cycle fatigue regime for an AA7075-T6 alloy. Subsequently, the model is validated via representative ultrasonic fatigue experiments for different stress levels that verified the estimation of fatigue crack formation in simulations. The study provides insights into various factors responsible for forming fatigue cracks in the material.

Next, the issue takes the reader to the second group of contributions that utilize modern *ab initio* or first principles methods to study and design a range of functional materials. The article by Hartman et al. [17] demonstrates the capability of first principles methods to design and screen materials for future valleytronics applications using a specific example of stacked two-dimensional heterointerfaces. In particular, it is shown that the interlayer band hybridization plays a major role in these systems when the bands associated with the two layers forming the interface are closely aligned in energy. Moreover, the resulting band repulsion and the total valley splitting are found to strongly depend on the on-site Coulombic repulsion captured by the Hubbard correction. The contribution by Karabin et al. [18] presents a comparative study of different modeling approaches (namely, the special quasi-random structures modeling, the multiple-scattering single-site coherent potential approximation, and the locally self-consistent multiple-scattering method) to the electronic properties of the $Hf_{0.05}Nb_{0.05}Ta_{0.8}Ti_{0.05}Zr_{0.05}$ high entropy alloy. While their analysis reveals no signature for the long-range or local magnetic moments formation in the alloy, their results indicate the presence of possible superconductivity below 9 K. Closely aligned with the theme, the paper by Kumar et al. [19] employs density functional theory and Boltzmann transport equations to study structural, elastic, electronic, and thermoelectric properties of a tetragonal Zintl compound, $RbZn_4P_3$, highlighting its potential as a thermoelectric energy harvesting material. The articles by Mehta et al. [20] and Vemuri et al. [21] focus on two-dimensional functional

materials. While the former contribution investigates electrochemical performance of double transition metal MoWC MXene for its potential usage as an efficient anode material in Li-ion batteries, the latter study presents a novel route to develop highly conductive graphene sheets using camphor as a natural precursor followed by nitrogen doping via low temperature post-annealing treatment and further rationalizes the effect of nitrogen doping on the electrical properties of the material. The last contribution in this group from Panneerselvam et al. [22] is focused on understanding the photophysical effects of hydroxyl (–OH) substitution at the different positions on phenyl rings in pyrene-based Schiff base derivatives of 4-[(pyren-1-ylmethylene)amino]phenol (PAP). Utilizing density functional theory and time-dependent density functional theory methods, this study compares the configuration-dependent relative electronic effects of different PAP isomers to identify potential candidates as fluorescent probe for diverse applications.

The last group of articles highlights contributions falling within multiple categories, including data-enabled machine learning methods, numerical modeling, and high throughput computational screening of potentially effective therapeutic candidates for the infectious disease Coronavirus 2019 (COVID-19). The article by Mannodi-Kanakkithodi et al. [23] tackles an exciting problem that concerns developing predictive machine learning models to predict formation energies and charge transition levels of substitutional defects in methylammonium lead halide perovskites to identify optoelectronically active impurity atoms. This approach enables predictions for hundreds of impurities across a range of host chemistries to identify impurities that can shift the equilibrium Fermi level in the perovskite as determined by native point defects and, as a result, provides an alternative route towards efficient screening of impurities that may cause undesired recombination of charge carriers, or enable an effective tuning of the host conductivity and resulting photovoltaic absorption. The article by Geng et al. [24] reports development of a data-driven machine learning model to predict the hardenability curve of high-strength boron steel. Subsequently, the validated model is combined with an experimental design approach to first predict and then successfully synthesize a new boron steel composition with improved hardenability. The article by Lin et al. [25] utilizes numerical methods to understand the effects of different parameter in ultrasonic-assisted electric discharge methods on the resulting particle size distribution of the metallic powders produced, providing valuable guidance toward the design and preparation of metallic powders. Finally, the article by Kashyap et al. [25] presents a multi-step hierarchical down-selection strategy to address an important contemporary challenge of identifying potentially effective therapeutic candidates for COVID-19. More specifically, the computational approach combining high throughput molecular docking, molecular dynamics analysis, and density functional theory analysis is used to identify three distinct ligands attacking different binding sites of the same protein (7BV2) of SARS-CoV-2, which can potentially increase the probability of the candidates surviving an in vivo trial.

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References

[1] Curtarolo S, Hart GL, Nardelli MB, Mingo N, Sanvito S, Levy O (2013) The high-throughput highway to computational materials design. Nat Mater 12(3):191–201

[2] Martin RM (2020) Electronic structure: basic theory and practical methods, Cambridge university press

[3] Marx D, Hutter J (2009) Ab initio molecular dynamics: basic theory and advanced methods, Cambridge University Press

[4] Butler KT, Davies DW, Cartwright H, Isayev O, Walsh A (2018) Machine learning for molecular and materials science. Nature 559(7715):547–555

[5] Ramprasad R, Batra R, Pilania G, Mannodi-Kanakkithodi A, Kim C (2017) Machine learning in materials informatics: recent applications and prospects. .pj Comp Mater 3(1):1–13

[6] Bartel CJ (2022) Review of computational approaches to predict the thermodynamic stability of inorganic solids. J Mater Sci, 1–2
[7] Uberuaga BP, Simonnin P, Rosso KM, Schreiber DK and Asta M (2022) The effect of Cr alloying on defect migration at Ni grain boundaries. J Mater Sci, 1–18
[8] Sose AT, Mohammadi E, Wang F, and Deshmukh SA (2022) Investigation of structure and dynamics of water confined between hybrid layered materials of graphene, boron nitride, and molybdenum disulphide. J Mater Sci, 1–18
[9] Nikolov S, Tranchida J, Ramakrishna K, Lokamani M, Cangi A, and Wood M (2022) Dissociating the phononic, magnetic and electronic contributions to thermal conductivity: a computational study in alpha-iron. J Mater Sci, 1–14
[10] Mishra A, Echeverria MJ, Ma K, Parida S, Chen C, Galitskiy S and Dongare AM (2022) Virtual texture analysis to investigate the deformation mechanisms in metal microstructures at the atomic scale. J Mater Sci, 1–20
[11] Gupta AK, Gohil S (2022) Insights into structural difference between sodium polyacrylate PAA and sodium polymethacrylate PMA in salt solutions investigated by molecular simulations. J Mater Sci, 1–16
[12] Fey LT, Hunter A and Beyerlein IJ (2022) Phase-field dislocation modeling of cross-slip. J Mater Sci, 1–15
[13] Coutinho YA, Kunwar A and Moelans N (2022) Phase-field approach to simulate BCC-B2 phase separation in the AlnCrFe2Ni2 medium-entropy alloy. J Mater Sci, 1–13
[14] Siddique AB and Khraishi TA (2022) Multi-scale modeling of solute atom strengthening using 3D discrete dislocation dynamics. J Mater Sci, 1–14
[15] Izvekov S, Larentzos JP, Brennan JK and Rice BM (2022) Bottom-up coarse-grain modeling of nanoscale shear bands in shocked α-RDX. J Mater Sci, 1–22
[16] Li B, Gao T, Xue H and Sun Z (2022) Estimation of fatigue crack initiation in the very high cycle fatigue regime for AA7075-T6 alloy using crystal plasticity finite element method. J Mater Sci, 1–15
[17] Hartman ST and Pilania G (2022) Strong Zeeman splitting in orbital-hybridized valleytronic interfaces. J Mater Sci, 1–13
[18] Karabin M, Mondal W, Ostlin A, Ho W-GD, Dobrosavljevic V, Tam K-M, Terletska H, Chioncel L, Wang Y and Eisenbach M (2022) Ab initio approaches to high entropy alloys: a comparison of CPA, SQS, and Supercell Methods. J Mater Sci.
[19] Kumar R, Singh M et al (2022) Realizing high thermoelectric performance in p-type RbZn4P3 Zintl compound: a first-principles investigation. J Mater Sci, 1–11
[20] Mehta V, Saini HS, Srivastava S, Kashyap MK and Tankeshwar K (2022) Ultralow diffusion barrier of double transition metal MoWC monolayer as Li-ion battery anode. J Mater Sci, 1–12
[21] Vemuri SK, Chaliyawala H, Ray A and Mukhopadhyay I (2022). A powerful approach to develop nitrogen-doped graphene sheets: theoretical and experimental framework. J Mater Sci, 1–10
[22] Panneerselvam M, Kathiravan A, Johnee Britto N, Krishnan SM, Velmurugan G and Jaccob M (2022) Delineating the effect of substituent and π-bridge flip on the photophysical properties of pyrene derivatives: answers from DFT/TD-DFT calculations. J Mater Sci, 1–12
[23] Mannodi-Kanakkithodi A and Chan MK (2022) Accelerated screening of functional atomic impurities in halide perovskites using high-throughput computations and machine learning. J Mater Sci, 1–19
[24] Geng X, Cheng Z, Wang S, Peng C, Ullah A, Wang H and Wu G (2022) A data-driven machine learning approach to predict the hardenability curve of boron steels and assist alloy design. J Mater Sci, 1–14
[25] Lin F, Liu Y, Song X, Liu X and Li X (2022) The numerical research on the effect of ultrasonic field on metallic powders produced by the ultrasonic-assisted electrical discharge process. J Mater Sci, 1–11
[26] Kashyap J and Datta D (2022) Drug repurposing for SARS-CoV-2: a high-throughput molecular docking, molecular dynamics, machine learning, and DFT study. J Mater Sci, 1–23