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Preface on Novel Aspects in Theoretical and Computational Surface Science (NATCSS)

Recent advancements in surface science, particularly in theoretical and computational approaches, have significantly deepened our understanding of fundamental aspects. The rapid evolution of high-performance computers has propelled the application of computational methods, enabling the simulation of complex phenomena with greater accuracy. The integration of artificial intelligence (AI), data mining, and other computational theories has further driven this computational revolution. Theoretical and computational surface science aims to predict desirable properties and understand surfaces and interfaces, contributing crucially to solving complex scientific problems. This Special Issue, titled "Novel Aspects in Theoretical and Computational Surface Science (NATCSS)," explores various computational techniques such as density functional theory (DFT), molecular dynamics (MD), Monte Carlo (MC) method, and machine learning (ML) approaches, addressing both inorganic and organic surfaces, and hybrid interfaces with potential industrial applications.

A. Sengupta investigated the Li adsorption properties of a hybrid 2D material, B_5Se, using first-principles calculations. Their study revealed that B_5Se has a distorted hexagonal structure with favorable cohesive energy and a metallic nature. The material demonstrated promising characteristics as an anode for Li-ion batteries, with a maximum theoretical specific capacity of 1486.87 mAh g^{-1}, significantly surpassing conventional anode materials. These properties make B_5Se a potent candidate for next-generation battery applications.

Axel Groß examined the behavior of oxygen atoms on stepped platinum surfaces using an ab initio molecular dynamics simulations. Their study challenges the traditional view that chemical reactions are solely governed by thermodynamics. By investigating hot atom dynamics, they provide insights into reaction mechanisms that occur on catalytic surfaces, which could lead to improved design and optimization of catalytic processes.

Attia Batool and colleagues explored the potential of tin monochalcogenides (SnSe, SnS) for use in Li-ion batteries, optoelectronics, sensors, and thermoelectric applications. Utilizing DFT, they examine the electronic, optical, and structural properties as these materials transition from bulk to monolayer or bilayer structures. Their findings indicate that as the thickness of the material increases, its isotropic behavior and crystallinity also increase. This research provides valuable insights into the tunable properties of tin monochalcogenides, paving the way for their application in various energy storage and optoelectronic devices.

Nguyet N. T. Pham studied the unique electronic and structural properties of bilayer graphdiyne (GDY), focusing on its potential in electrocatalytic applications. The research compares pristine and N-doped bilayer GDY, revealing that N-doping decreases the energy gap and enhances the thermodynamic stability, particularly at the *sp*-N_2 site in AB(β1) and AB(β2) stacking models. The study finds that while N-doped GDY shows limited selectivity for toxic gases like CO, CO_2, and HCHO, it demonstrates promising activity for oxygen reduction, making it a potential candidate for CO-tolerant electrocatalyst systems.

N. P. Barde and colleagues synthesized lithium ferrite nanoparticles dispersed in a silica matrix using an ultrasonic-assisted sol-gel method, revealing significant changes in the material's properties. The dispersion of nanoparticles in silica reduced agglomeration, modifying surface characteristics and enhancing system performance. X-ray diffraction confirmed a simple cubic spinel structure, and dynamic magnetic field susceptibility studies showed a dominance of reversible magnetic domain walls. The study found that increasing silica content led to a reduction in optical and dielectric properties, such as refractive index and optical basicity, while dielectric polarizability and other parameters increased. These findings suggest that fine-tuning the silica content can optimize the material's properties for various applications.

A. H. Omranpoor and colleagues conducted ab initio molecular dynamics simulations to explore how temperature, surface structure, and electrochemical environment affect the oxidation of 2-propanol to acetone at the Co_3O_4 (001)/H_2O interface. The study revealed that 2-propanol adsorbs differently on A-terminated and B-terminated surfaces, which vary in the number of Co^{2+} and Co^{3+} ions. At room temperature, no C-H bond cleavage occurs, but under oxidative conditions, dehydrogenation of the alcoholic OH group leads to the formation of 2-propanolate, which further reacts on the B-terminated surface to produce acetone. The presence of adsorbed hydroxyl groups aids in proton transfer, facilitating the reaction, while increasing the temperature to 450 K does not result in C-H bond dehydrogenation, highlighting the importance of the electrochemical environment in the oxidation process.

Fabrizio Bettetti and colleagues provide a comprehensive review of existing models for adsorption-desorption noise in bio-chemical sensors, focusing on models derived from the forward Kolmogorov equation and those based on Langevin sources. They propose a generalized model to address complex scenarios, such as branched surface reactions and chained reactions. The study benchmarks these models against kinetic Monte Carlo (kMC) simulations, examining cases like pH-sensitive ions and multi-layer adsorption. The results demonstrate that, despite differences in mathematical formulations, the models are equivalent when applied to independent binding sites, showing a perfect match with kMC results. Additionally, the study explores competitive binding scenarios, analyzing the impact of correlated binding site occupation.

Chia-Chi Chang and colleagues employed DFT to design and analyze innovative electrocatalysts for the electrochemical CO_2 reduction reaction (ECRR). Their study focused on single-metal dual site catalysts (SM-

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DSCs) based on monolayer boron nitride (BN) modified with silicon (Si) or carbon (C) coordinating atoms. The results indicated that Fe@BN_Si(B) and Fe@BN_C(N) configurations were the most stable and demonstrated high selectivity for CO_2 reduction over the hydrogen evolution reaction (HER). Fe@BN_Si(B) exhibited a lower limiting potential of –0.63 V, making it a promising candidate for efficient CO_2 reduction. Additionally, introducing water co-adsorption reduced the required potential further, highlighting the potential for enhancing catalytic performance.

Chen Wang and colleagues conducted a first-principles study to examine the characteristics of the crystalline-amorphous W/B_4C interface. They modeled three amorphous B_4C structures combined with various tungsten (W) layers to establish W/α-B_4C interfaces, analyzing properties such as adhesion work, electronic structure, and tensile mechanical properties. The study found that the W(200)/α-$B_{11}C_p$-CBC interface exhibited the strongest atomic bonding and highest adhesion work, though it experienced atomic reconstruction under strain. In contrast, the W(110)/α-B_{top}-$B_{11}C_p$-CBC interface maintained excellent stability and combined both toughness and plasticity with a maximum tensile strength of 26.7 GPa. The research suggests that interface tensile strength is influenced by factors beyond adhesion work, including interfacial bonding characteristics.

Dexin Wang and colleagues utilized molecular dynamics simulations, X-ray diffraction, and scratch testing to investigate the crystallization behavior of amorphous cobalt (Co) under thermal conditions and its effects on the cohesive strength of WC/Co coatings. The study revealed that heat treatment prompted a phase transition from amorphous-Co to the η-phase, enhancing the coating's performance by increasing its cohesive strength. However, this treatment also led to a reduction in the ideal fracture energy (W_{sep}) after reaching 873 K, indicating a decrease in cohesive strength due to elastic strain during the early stages of η-phase nucleation. The findings underscore the complex impact of thermal treatment on the microstructural properties of the interface, highlighting the balance between improving mechanical properties and managing the detrimental effects of early-phase transformations.

In summary, this special issue highlights the detailed exploration of electronic, structural, and mechanical properties at the atomic and molecular levels, these studies offer insights into optimizing materials for energy storage, catalysis, and environmental sustainability. By employing computational, experimental, and theoretical methods, this issue underscores the critical role of interface characteristics in enhancing the performance and efficiency of technologically relevant materials. We are very pleased to serve as Guest Editors on this thematic issue involving ten high quality studies. We would like to express our gratitude to the Editorial staff of Applied Surface Science Advances for the invitation and continuous support. We are also most appreciative to all authors and reviewers for their efforts towards obtaining the current special issue.

Seung Geol Lee[a,*], Ian Shuttleworth[b], Herbert M. Urbassek[c], Byungchan Han[d], Alfredo Juan[e]

[a] *Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea*
[b] *School of Science and Technology, Nottingham Trent University, Nottingham NG11 8NS, UK*
[c] *Physics Department, University Kaiserslautern, Erwin-Schroedinger-Strasse, D-67663 Kaiserslautern, Germany*
[d] *Yonsei University, Yonsei-ro Seodaemun-gu, Seoul 03722, Republic of Korea*
[e] *Universidad Nacional del Sur, Av. Alem 1253, Bahia Blanca 8000, Argentina*

[*] Corresponding author.
E-mail address: seunggeol.lee@unist.ac.kr (S.G. Lee).