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# Energetics and Dynamics of Molecules, Solids and Surfaces

In this Special Section on Energetics and Dynamics of Molecules, Solids and Surfaces, a broad range of physical chemistry multidisciplinary areas are involved, i.e., theoretical/computational, experimental/technological methods. This section is special, however, in that it highlights, without being comprehensive or selective, some of the science from South America and especially Brazil. All submitted papers were peer-reviewed following the high scientific standards of *The Journal of Physical Chemistry* All contributing authors thank the Journal for this opportunity.

We summarize herewith the work presented in this special section.

A theoretical study on the nitration of methane by acyl nitrate catalyzed by HZSM-5 zeolite is reported. The calculations were performed at the DFT/X3LYP/6-31G** and MP2/6-31G** levels. The mechanisms involving the protonation of the acyl nitrate by the zeolite and the formation of a nitronium-like ion as well as the activation energies of these reactions are investigated.

Different origins of green-light photoluminescence emission in structurally ordered and disorder powders of calcium molybdate were investigated. X-ray diffraction, Raman spectroscopy, transmission electron microscopy images and density functional calculations were used to study these materials.

Plane-wave density functional calculations of crystallites formed of 100−200 transition metal atoms were used to mimic larger experimentally treated particles. A series of model Pd clusters containing up to 225 atoms is chosen as an example, focusing on the description of size-dependent geometric parameters, binding energies of these clusters as compared with previous benchmark calculations and evolution of the particle electronic structure with increasing size.

Density functional studies were made of the structural and electronic properties of low index rutile surfaces for $TiO_2/SnO_2/TiO_2$ and $SnO_2/TiO_2/SnO_2$ composite systems. Comparisons with the bare rutile structure, other theoretical calculations and experimental data were made.

The emission of wide band photoluminescence in barium zirconate and barium titanante thin films in alternate multilayer systems was investigated by experimental and theoretical methods to establish correlations between structural and optical properties of these multilayered systems.

The influence of structural disorder on the photoluminescence of $Pb(Zr_{0.53}Ti_{0.47}O_3)$ powders was investigated and correlated with the coordination modes of Ti.

A combined experimental and theoretical study was made toward a better understanding of intermediate and short-range defects in ZnO single crystals, i.e., symmetry breaking and creation of localized electronic levels.

The structural and electronic properties of ZnO surfaces were investigated by means of periodic density functional calculations.

The breathing orbital valence bond trial wave functions for diffusion Monte Carlo was applied to the computation of the carbon−hydrogen (C−H) bond dissociation energy of acetylene and compared with other theoretical results.

Density functional theory was used to study the adsorption of formaldehyde on $Pd_4$ and on $Pd_4/\gamma\text{-}Al_2O_3$ clusters and compared with experimental results. NBO analysis was made of the interaction between the formaldehyde and the $Pd_4$ supported clusters.

Molecular dynamics, density functional theory, virtual screening, ADMET predictions and molecular interaction field studies were used for studying novel potential inhibitors of CDK2 inhibitors in cancer therapy.

The adiabatic finite-nuclear-mass-correction to the electronic energies and wave functions of atoms and molecules is formulated for density-functional theory and the approach is tested for a series of local and gradient corrected density functionals, using MP2 results as standards and applied to obtain the adiabatic correction for full atomization of alcanes.

Polymer electrolytes were obtained by the casting technique and the membranes with good ionic conductivity properties were characterized by various experimental techniques.

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*Guest Editor*

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