Mojtaba Alaei

Department of Physics,

Isfahan University of Technology,

Isfahan, Iran

Title:

Calculation of exchange coupling constants using density functional theory

عنوان:

محاسبه‌ی ثابت‌های تبادلی با استفاده از نظریه تابعی چگالی

چکیده:

ثابت‌های تبادلی مانند ثابت‌های تبادلی هایزنبرگ، نقش تعیین کننده‌ای در نظم‌های مغناطیسی دارند. در آزمایشگاه معمولا بدست آوردن این ثابت‌های میکروسکوپی چالش برانگیز است. با محاسبه‌ی انرژی کل در نظریه‌ی تابعی چگالی برای پیکربندی‌های مختلف مغناطیسی می‌توان نتایج مربوط به این پیکربندی‌ها را به یک هامیلتونی مدل نگاشت کرد و به دین ترتیب ثابت‌های تبادلی مورد نظر را بدست آورد. در اینجا ما قصد داریم این شیوه محاسباتی خود را برای دو سیستم FeF_3 و $Bi_3Mn_4O_{12}(NO_3)$ با جزئیات توضیح دهیم و نتایج بدست آمده را با استفاده از شبیه سازی مونت کارلو (اسپینی) با نتایج آزمایشگاهی مقایسه کنیم.

Reza Asgari

Institute for Research in Fundamental Sciences,

Tehran, Iran

Title:

Quantum non-local effects in graphene plasmonics

Abolfazl Bayat

University College London,

London, England

Title:

A quantum information recipe for both quantum phase transitions and many-body localization

Karsten Kruse

Swiss National Center of Competence in Research Chemical Biology,

University of Geneva,

Geneva, Switzerland

Title:

Actin-wave driven migration - chance and necessity

Abstract:

Cell crawling on solid substrates is commonly characterised by protrusions that appear seemingly randomly along the cell periphery and drive the cell forward. This can result in erratic motion in form of a persistent random walk. It has been proposed that these protrusions are initiated and coordinated through spontaneous actin waves. Based on known molecular processes for actin-filament nucleation and negative feedback from the filaments onto the nucleating proteins, we develop a deterministic framework for studying actin polymerisation waves. We use a phase-field approach to study the possible impact of these waves on migration. We find that they can generate various migration patterns. Among them are notably erratic trajectories. We compare the computed trajectories to those obtained from live cell imaging. Our results show that spontaneous actin dynamics can lead to observed migration patterns, which offers cells a simple way to adapt to the topography of the surrounding environment and to respond to external cues.

Joerg Meyer

Leiden Institute of Chemistry,

Leiden University,

Leiden, The Netherlands

Title:

Modeling heat dissipation at the nanoscale: A tale about exciting electrons and phonons

Abstract:

Energy conversion at interfaces is at the centre of the rapidly growing field of basic energy science. Engineers routinely deal with important consequences on a macroscopic scale based on well-known continuum theories relying on empirically determined effective parameters, for which an atomistic understanding is very limited at best. Being an experimentally accessible observable, the vibrational lifetime of small adsorbates can provide detailed information about the energy exchange with the substrate at the atomic scale [1].

One dissipation channel that has received a lot of attention recently is given by the (electronically nonadiabatic) excitation of electron-hole pairs [2]. High-level non-adiabatic calculations beyond the ubiquitous Born-Oppenheimer approximation are, unfortunately, either conceptually challenging or computationally intractable for extended metal surfaces. Therefore, numerically appealing electronic friction schemes have attracted significant interest. By application to the vibrational damping of the CO adsorbed on Cu(100) and on Pt(111) surfaces, I will compare different ways to calculate the electronic friction tensors and concomitant approximations [3]. A perturbative approach rooted in time-dependent density functional theory (see [4] and references therein) allows us to go beyond the Markov approximation inherent to all current electronic friction theories and thus to scrutinize the influence of electronic coherence [5].

The other most prominent dissipation channel is given by vibrations of the surface lattice. State-of-the-art theory for describing this phononic dissipation mechanism is based on an elastic continuum model for the substrate, implicitly relying on harmonic solid [6]. This completely neglects temperature effects, thus hampering direct comparisons to experimental data. Given this situation we have developed a phonon projection scheme (see [7] and references therein) that allows to directly calculate vibrational lifetimes of adsorbate modes at finite temperature from non-equilibrium molecular dynamics simulations. Application to Na adsorbed on the Cu(100) surface shows that the lifetime of the frustrated translational mode is largely affected by surface temperature. We can explain this dependence on the basis of a simple model disentangling harmonic and anharmonic contributions [8].

Aiming at multiscale modeling of energy dissipation during chemical reactions at surfaces, I will finally discuss two new techniques to accurately account for phonon excitations in this context. First, our novel QM/Me approach [7,9] extends the power of embedding techniques to metallic systems. A huge atomistically described bath can thus be included in ab initio molecular dynamics simulations of chemical reactions at catalyst surfaces. Application to the

dissociation of O2 on Pd(100) predicts translationally “hot” oxygen adsorbates as a consequence of the released adsorption energy (ca. 2.6 eV). This questions the instant thermalization of reaction enthalpies generally assumed in models of heterogeneous catalysis [9]. Second, for N2 on Ru(0001) we have recently demonstrated that the molecule-surface interaction potential including phononic degrees of freedom can be represented accurately with ab initio quality by a high dimensional neural network. This reduces the computational cost of molecular dynamics calculations by several orders of magnitudes and thus allows for reaction probabilities as low as 10−5 to be computed for this system – in good agreement with experimental data [10].

References

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Saman Moghimi

Department of Physics,

Sharif University of Technology,

Tehran, Iran

Title:

Critical self-organization, sand hills and neural science

عنوان:

خودساماندهی بحرانی، تپه های شنی و علوم اعصاب

چکیده:

عمدتا خواص بحرانی در مواد با تنظیم پارامترهای خارجی، مانند دما یا میدان‌های بیرونی به وجود می آید. اما در طبیعت نمونه های فراوانی دیده می شود که در آن ها بدون تنظیم پارامترهای بیرونی، سیستم حالت بحرانی از خود بروز می دهد. زلزله ها، آتش سوزی ها و ارتفاع کوه ها از این دسته هستند. مدل‌های ساده سازی شده ای برای توصیف این پدیده ها ارایه شده است که مهمترین آنها مدل تپه های شنی است. خواص متعدد این مدل و مدل های مشابه مورد بررسی قرار گرفته است. در این ارایه سعی می کنم این خواص را برشمرم و نشان دهم با چه مکانیسمی می توان این سیستم‌ها را از حالت بحرانی دور کرد. علاوه بر این، ارتباط این مدل با علوم اعصاب و مغز را مورد توجه قرار می دهم.

Farshid Mohammad Rafiee

Department of Physics,

Institute for Advance Studies in Basic Sciences (IASBS),

Zanjan, Iran

Title:

Some biophysical aspects of translation process in protein synthesis

Shahpoor Saeidian

Department of Physics,

Institute for Advance Studies in Basic Sciences (IASBS),

Zanjan, Iran

Title:

Few-body physics of quasi-one dimensional atomic gases

Abstract:

We investigate a theoretical method to study the quantum dynamics of ultracold atomic gases inside an atomic waveguide with harmonic confinement. For quasi-1D gases, the confining potential of the waveguide leads to the so-called confinement induced resonance (CIR). In the vicinity of CIR, the atom-atom coupling strength g_1D diverges, results in the phase transition of the bosonic gas to the impenetrable regime (known as TG gas). In this regime the bosons repel each other strongly and behave like fermions. We analyze the elastic as well as inelastic multi-channel confined scattering. For the elastic scattering, the effects of the interatomic potential and the waveguide anisotropy on the width and position of the CIR are studied. Furthermore, we investigate the thermodynamics of quasi-1D atomic gases across wide and narrow CIR. Universal thermodynamics is identified for the repulsive scattering branch right at the wide CIR. At narrow CIR this is washed away by the strong energy dependence of the coupling strength.

Seyed-Nader Seyed-Reihani

Department of Physics,

Sharif University of Technology,

Tehran, Iran

Title:

Examination of biological tissues using optical tweezers