
3rd IRISH ATOMISTIC SIMULATION CONFERENCE

to be held at

UNIVERSITY COLLEGE CORK

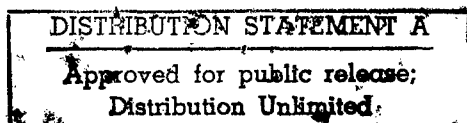
DECEMBER 21-22, 1998

CONFERENCE SCHEDULE

Venue: All talks will be held in Room G7 of the Robert Kane (Science) Building, University College Cork, main campus.

Monday, December 21

- 2:30pm start of conference
- 2:35pm
Michael Nolan, NMRC Molecular Dynamics Simulations of the Phase Transitions of the Homopolymer of p-hydroxybenzoic Acid
- 3:05pm
Don MacElroy, UCD Molecular simulation of the separation of gas mixtures using thin nanoporous membranes
- 3:50-4:20pm coffee break
- 4:20pm
Paul Smith, QUB An investigation into surface ordering in liquid n-alkanes with molecular dynamics.
- 4:50pm
Paddy Kane, DCU Conformational Analysis of Complexes of Phosphine Oxide Calix-[4]-arenes with Group 1 and Group 2 Cations
- 5:20pm
Charles Patterson, TCD GW Calculations in a Gaussian Orbital Basis
- 8:30pm — Conference Dinner at Proby's Bistro, Proby's Quay, Cork



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AQF9906-1081

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE 1999	3. REPORT TYPE AND DATES COVERED Conference Proceedings	
4. TITLE AND SUBTITLE 1998 Irish Atomistic Simulators Meeting			5. FUNDING NUMBERS F61775-99-WF006	
6. AUTHOR(S) Conference Committee				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) National Microelectronics Research Center (NMRC) Lee Maltings, Prospect Row Cork Ireland			8. PERFORMING ORGANIZATION REPORT NUMBER N/A	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) EOARD PSC 802 BOX 14 FPO 09499-0200			10. SPONSORING/MONITORING AGENCY REPORT NUMBER CSP 99-5006	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.			12b. DISTRIBUTION CODE A	
13. ABSTRACT (Maximum 200 words) The Final Proceedings for 1998 Irish Atomistic Simulators Meeting, 16 December 1998 - 17 December 1998 This is an interdisciplinary conference. Topics include computation of material properties including polymer and bio-polymer simulation, electronic spectra and polarizations of solids.				
14. SUBJECT TERMS EOARD, Materials, Semiconductor materials			15. NUMBER OF PAGES 7	16. PRICE CODE N/A
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

Tuesday, December 22

9:00am

Stephen Fahy, UCC Infrared absorption as a probe of strain and microstructure in boron nitride thin films

9:30am

Isakander Batyrev, QUB First principles simulation of the work of adhesion of Nb(111)-/Al₂O₃(0001) interface

10:00am

Jim Greer, NMRC Atomistic simulation and ab initio computations for microelectronics

10:30am

A. Michaelides, QUB Why is subsurface hydrogen more reactive than surface hydrogen in catalytic hydrogenation?

11:00–11:20am

coffee break

11:20am

Michael Kuzmin, TCD Onset of Magnetic Order in Ferromagnetic Nanostructures.

11:50am

Mike Finnis, QUB Modelling oxides: simplifications from ab initio density functional theory

12:25pm

Mike Harris, UCC QMC for excited collective states

Affiliations of Speakers:

Isakander Batyrev Atomistic Simulation Group, Queens University, Belfast.
Stephen Fahy Department of Physics, University College, Cork.
Mike Finnis Atomistic Simulation Group, Queens University, Belfast.
Jim Greer Materials Modelling Group, National Microelectronics Research Centre, UCC, Cork.

Mike Harris Department of Physics UCC, and Max-Planck Institute, Stuttgart.
Paddy Kane School of Chemical Sciences, Dublin City University.
Michael Kuzmin Department of Physics, Trinity College, Dublin.
Don MacElroy Department of Chemical Engineering, NUI, Dublin.
A. Michaelides Department of Chemistry, Queens University, Belfast.
Michael Nolan Materials Modelling Group, National Microelectronics Research Centre, UCC, Cork.

Charles Patterson Department of Physics, Trinity College, Dublin.
Paul Smith Atomistic Simulation Group, Queens University, Belfast.

ABSTRACTS OF PRESENTATIONS

Molecular Dynamics Simulations of the Phase Transitions of the Homopolymer of p-hydroxybenzoic Acid

Michael Nolan

Materials Modelling Group, National Microelectronics Research Centre, UCC, Cork.

We present the results of force-field calculations and molecular dynamics simulations on the homopolymer of the liquid crystal polymer p-hydroxybenzoic acid. A model unit cell with two chains and six monomers per chain was constructed based on experimental results. The FF calculations were used to optimise the lattice structure. The MD simulations were carried out within the NPT ensemble, allowing for changes in the cell parameters and shape. Discontinuities in the isobaric specific heat capacity as a function of temperature were used as the signature for the phase transitions. Good agreement with the experimentally quoted phase transitions was found. The structural changes which occur at the first phase transition were also modelled. We also present an analysis of the molecular motion which occurs at and determines each phase transition.

Molecular simulation of the separation of gas mixtures using thin nanoporous membranes

Don MacElroy

Department of Chemical Engineering, NUI, Dublin.

A nonequilibrium molecular dynamics (NEMD) simulation technique is employed to investigate the transport of binary mixtures of hydrogen and methane through a model carbon membrane of varying thickness. Both forced flow simulations under a pressure gradient and isobaric counterdiffusion simulations are described in this presentation. The principal conclusions of these studies are: (i) pore entrance/exit effects may need to be taken into consideration in membrane design for hydrogen/hydrocarbon separations if the length of the controlling pores within the carbon membrane is of the order of one tenth of a micron or less; (ii) viscous (convective) flow contributions to the fluxes of the individual components of the mixture should be negligible for the carbon membranes currently in use; and (iii) the cross-coefficients of diffusion appear to play a relatively minor role in the normal (pressure driven) hydrogen/methane membrane separation process however under isobaric conditions the simulation results suggest that hydrogen/methane cross-coupling plays a significant role in hindering the hydrogen counterdiffusion flux within carbon membranes containing long, narrow pores.

An investigation into surface ordering in liquid *n*-alkanes with molecular dynamics

Paul Smith

Atomistic Simulation Group, Queen's University, Belfast.

The unusual surface-ordered state of liquid *n*-alkanes was investigated by simulations of a slab of liquid heptadecane with two free surfaces. The results confirm that the surface-ordered state consists of a monolayer of molecules aligned perpendicular to the surface which are mostly in an all trans conformation. The local arrangement of molecules within the monolayer is hexagonal and the density is higher than in the bulk phase. Good agreement was found between the simulation results and X-ray diffraction and reflection data.

Conformational Analysis of Complexes of Phosphine Oxide Calix-[4]-arenes with Group 1 and Group 2 Cations

Paddy Kane, Kevin Kincaid, Darren Fayne and Dermot Diamond

School of Chemical Sciences, Dublin City University, Glasnevin, Dublin 9.

Monte Carlo conformational searches in combination with energy minimisation by molecular mechanics were used to model the complexes formed between two calixarenes, 1 and 2, and the Na⁺, Li⁺, K⁺, Mg²⁺ and Ca²⁺. ¹H NMR titrations were carried out to investigate the stoichiometry of the complexes and the structural changes which take place upon complexation. The mode of complexation for each complex is examined and the results are compared with the results of selectivity studies. 2 is known from potentiometric studies to be selective for Ca²⁺ in the presence of Li⁺, Na⁺ and Mg²⁺. ¹H NMR studies indicated that the 2:Ca²⁺ complex has a 1:1 stoichiometry. The modelling studies indicated that the Ca²⁺ ion was co-ordinated by the eight oxygen atoms of 2 and that this mode of complexation was unique for the 2 complexes. In contrast, an eight-fold mode of complexation was observed in the models of the complexes formed by 1 with three of the ions studied — Na⁺, K⁺ and Ca²⁺. These results clearly demonstrate why 2 shows a strong preference for calcium in the presence of the other interferents studied and also why 1 has a poor ability to discriminate between calcium and some of the other interferents.

GW Calculations in a Gaussian Orbital Basis

C.H. Patterson

Department of Physics, Trinity College, Dublin.

Hartree-Fock and Density Functional Theory methods applied to electrons in solids are well-known to result in band structures and other properties which differ from each other and from experiment. The usual problem is that the Hartree-Fock approximation results in band gaps that are too large and density functional theory results in gaps that are

too small, or non-existent. Hedin's GW method has been applied to semiconductors, insulators and metals in the last 12 years or so and generally gives a satisfactory account of the electronic structures of these materials. GW calculations in a Gaussian orbital basis are discussed as well as GW results for an insulator in the extreme tight-binding limit.

Infrared absorption as a probe of strain and microstructure in boron nitride thin films

Stephen Fahy

Department of Physics, University College, Cork.

Experimental and theoretical investigations of the infrared active, polarization dependent phonon frequencies of cubic boron nitride films have been performed [1] in light of recent claims that large frequency shifts during initial nucleation are the result of strain caused by highly non-equilibrium growth conditions. We show that the formation of small, separate grains of cubic boron nitride during the initial growth leads to a frequency shift in the infrared active transverse optic mode polarized normal to the substrate which is opposite in sign and twice the magnitude of the shift for modes polarized parallel to the substrate. In contrast, film strain causes a frequency shift in the mode polarized normal to the substrate which is much smaller in magnitude than the frequency shift for modes polarized parallel to the substrate. Normal and off-normal incidence absorption measurements, performed at different stages of nucleation and growth, show that large frequency shifts in the transverse optic phonon modes during the initial stage of growth are not compatible with the expected effects of strain, but are in large part due to nucleation of small isolated cubic BN grains which coalesce to form a uniform layer. Numerical results from a simple model of island nucleation and growth are in good agreement with experimental results.

[1] S. Fahy, C. A. Taylor, and R. Clarke, *Phys. Rev. B* **56**, 12573-80 (1997).

Atomistic simulation and ab initio computations for microelectronics

Jim Greer

Materials Modelling Group, National Microelectronics Research Centre, UCC, Cork.

In 1997, the NMRC, Ireland established a new unit within the Advanced Materials & Technology Group to apply material computation methods to problems of relevance to microelectronic issues. Material computation work represents a clear departure from the TCAD used within the microelectronics industry. The emerging use of ab initio and atomistic simulations for microelectronic applications reflects the fact that lateral dimensions of a few hundred nanometers and vertical dimensions of hundreds of angstroms are now routinely being manufactured. NMRC material computations have concentrated on application of molecular dynamics simulations to studies of liquid crystal polymers (see the

abstract by Mick Nolan in these proceedings), investigation of potential barriers at strained Si/SiGe interfaces, calculation of defects in compound semiconductors, software and application work on a Monte Carlo CI code, and newly we are moving into the area of quantum device simulation in collaboration with Physics, UCC. In this presentation, we will discuss the areas of application for ab initio and atomistic simulation in the microelectronics simulation hierarchy. Discussion of recent results obtained at the NMRC, and in particular, calculations of the carbon tetramer using the MCCI method will be presented.

Why is subsurface hydrogen more reactive than surface hydrogen in catalytic hydrogenation?

A. Michaelides

Department of Chemistry, Queen's University, Belfast.

In the catalytic hydrogenation of hydrocarbons, subsurface hydrogen has been experimentally demonstrated by Ceyer and co-workers to be much more reactive than surface hydrogen. We use density functional theory to identify low energy pathways for the hydrogenation of methyl adsorbed on Ni(111) by surface and subsurface hydrogen. The unique reactivity of subsurface hydrogen is found to be due to its excess potential energy rather than, as has previously been suggested, a more favourable transition state. The rate limiting step is the resurfacing of H. These features are expected to hold for other hydrogenation reactions.

Onset of Magnetic Order in Ferromagnetic Nanostructures

M.D. Kuzmin

Department of Physics, Trinity College, Dublin.

A simple phenomenological model is proposed, which describes two-component nanostructural ferromagnets. The entire space is divided into two domains filled with two distinct ferromagnetic media whose bulk Curie points are T_{c1} and T_{c2} , $T_{c1} > T_{c2}$. The two materials are assumed to grow into each other at the interface so that the exchange coupling across the interface has the same intensity as in the bulk. Importantly, the size of the high- T_c domain is restricted to a small value (d_1) in either 1, or 2, or 3 dimensions. The main result is that the ordering temperature of the system is lower than T_{c1} . The deviation from T_{c1} in the first non-vanishing approximation is quadratic in Δ/d_1 and independent from T_{c2} ($\Delta \approx 1\text{\AA}$ is a universal exchange length).

Modelling oxides: simplifications from ab initio density functional theory

Mike Finnis

Atomistic Simulation Group, Queen's University, Belfast.

I point out how the usual Hohenberg-Kohn-Sham total energy functional can be reformulated in a way that leads to the simplified models such as the ionic model and the tight-binding model. Tony Paxton and I derived a self-consistent tight-binding model [1] on this basis which we have applied to studying the phases of ZrO_2 .

[1] M.W. Finnis, A.T. Paxton, M. Methfessel and M. van Schilfgaarde, Phys. Rev. Letters, **81**, 5149-5152 (1998)

QMC for excited collective states

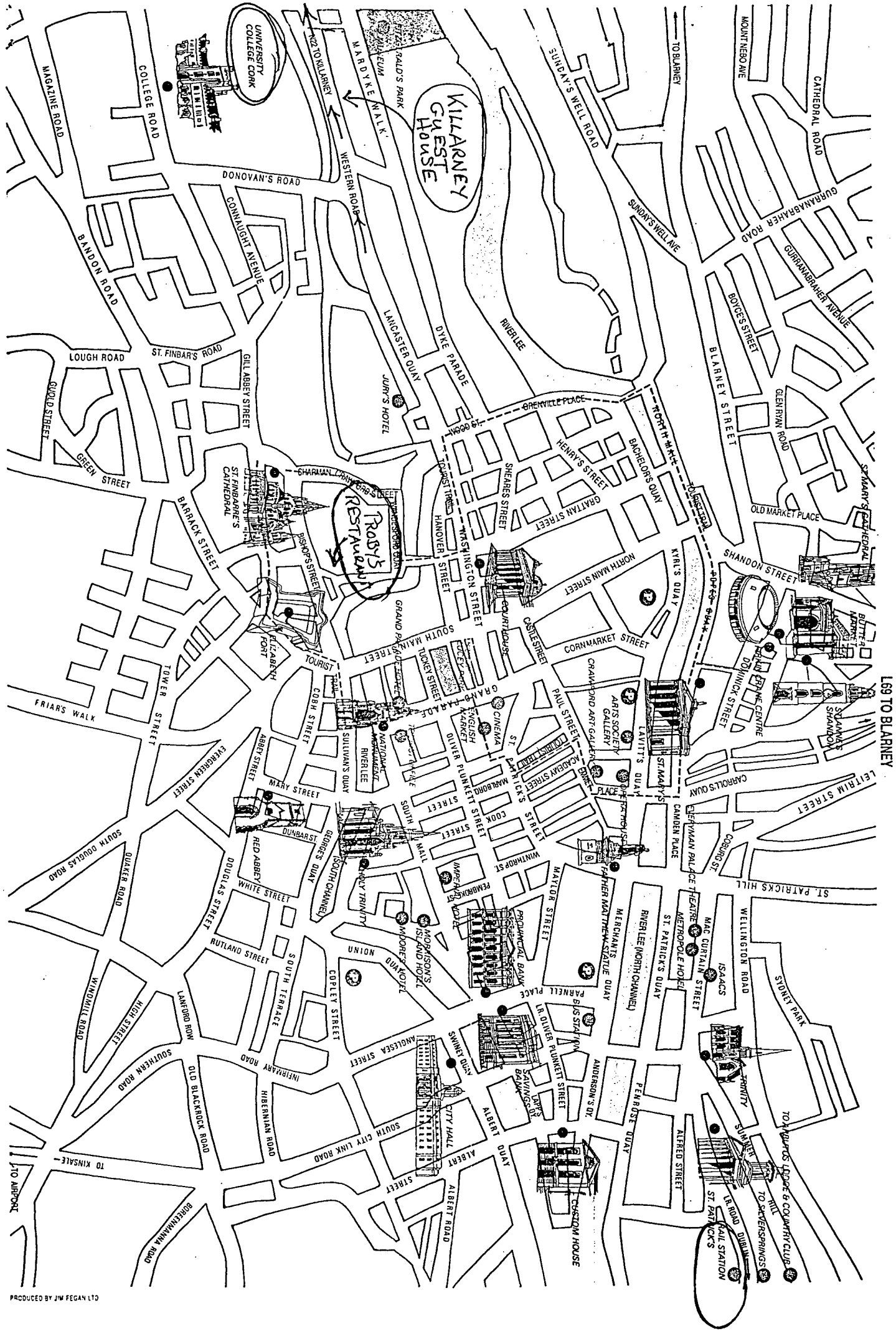
Mike Harris

Department of Physics, UCC, and Max-Planck Institute, Stuttgart.

Excitation spectra for the dipole and quadrupole plasma oscillations in jellium spheres are obtained by the analytic continuation of imaginary time correlation functions computed by the fixed node diffusion Monte Carlo method. The results provide benchmark data to test approximate theories for excited states (e.g., the random phase approximation, time dependent density functional and the GW method). The method is also applied to the calculation of the plasmon dispersion relations for both plasmon and spin wave excitations in the homogenous electron gas at various electronic densities.

We wish to thank the following for their contribution to the success of this conference:

United States Air Force Office of Scientific Research, European Office of Aerospace Research and Development.



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