Imperial College London QUPLA

QUANTUM PLASMONICS

QUPLA

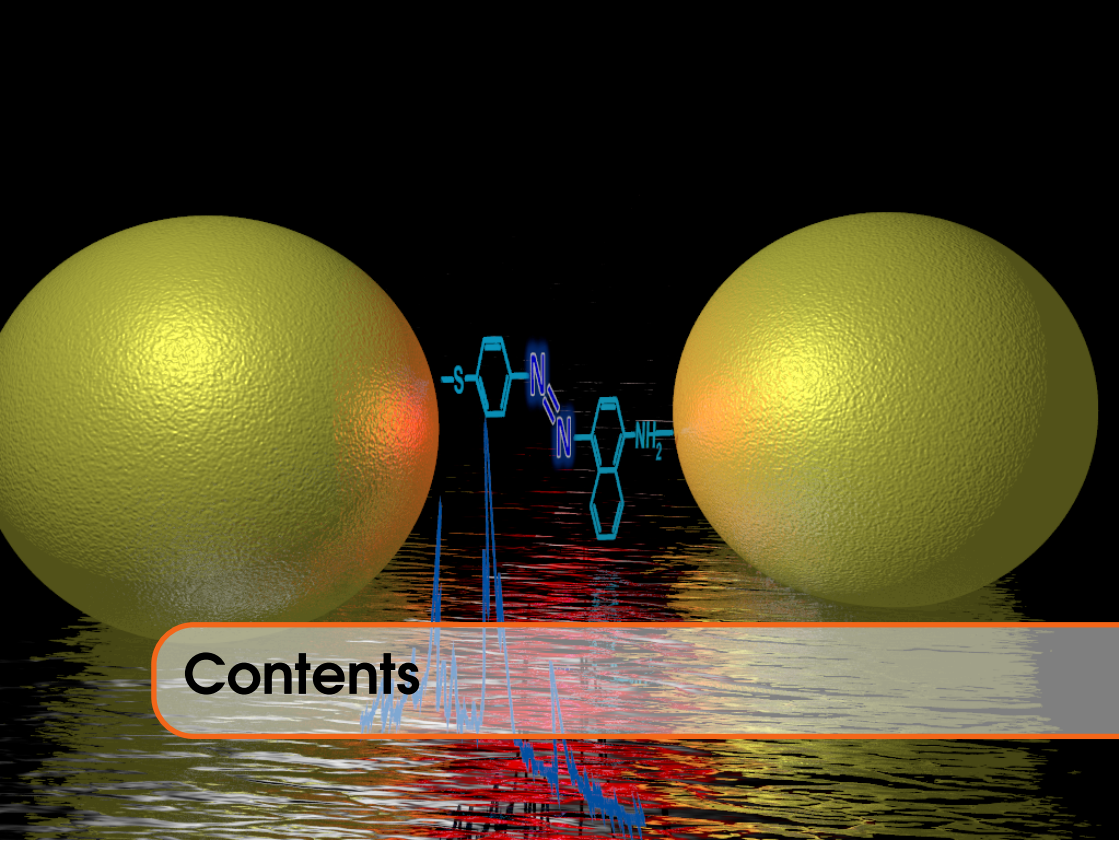
Welcome 1 — Goal. The main goal of QUPLA is to initiate a discussion and an exchange of ideas between researchers who model plasmonic systems, but work in different subfields of nanophysics. Specifically, the workshop will focus on light-matter interactions involving small metal nanoparticles and regimes when quantum effects are relevant and give rise to novel phenomena with potential for technological applications and advances in basic science. ■

In the last few years, mainly because of advances in nanofabrication, interest in plasmonics moved towards the properties of very small nanoparticles systems. In such systems, a new challenge arises, the appearance of quantum effects. In fact, until now, plasmonics has been mainly based on classical physics concepts.

Recently, there have been significant efforts to include quantum effects. Such approaches either modify the classical Maxwell equations of electrodynamics by introducing, for example, nonlocal, nonlinear and quantized fields or "borrow" quantization techniques used in empty cavities in quantum optics. However, such *ad hoc* approaches are fundamentally unsatisfactory and novel, microscopically accurate description of plasmonic systems that includes quantum effects is sorely needed.

The organiser, August 2016

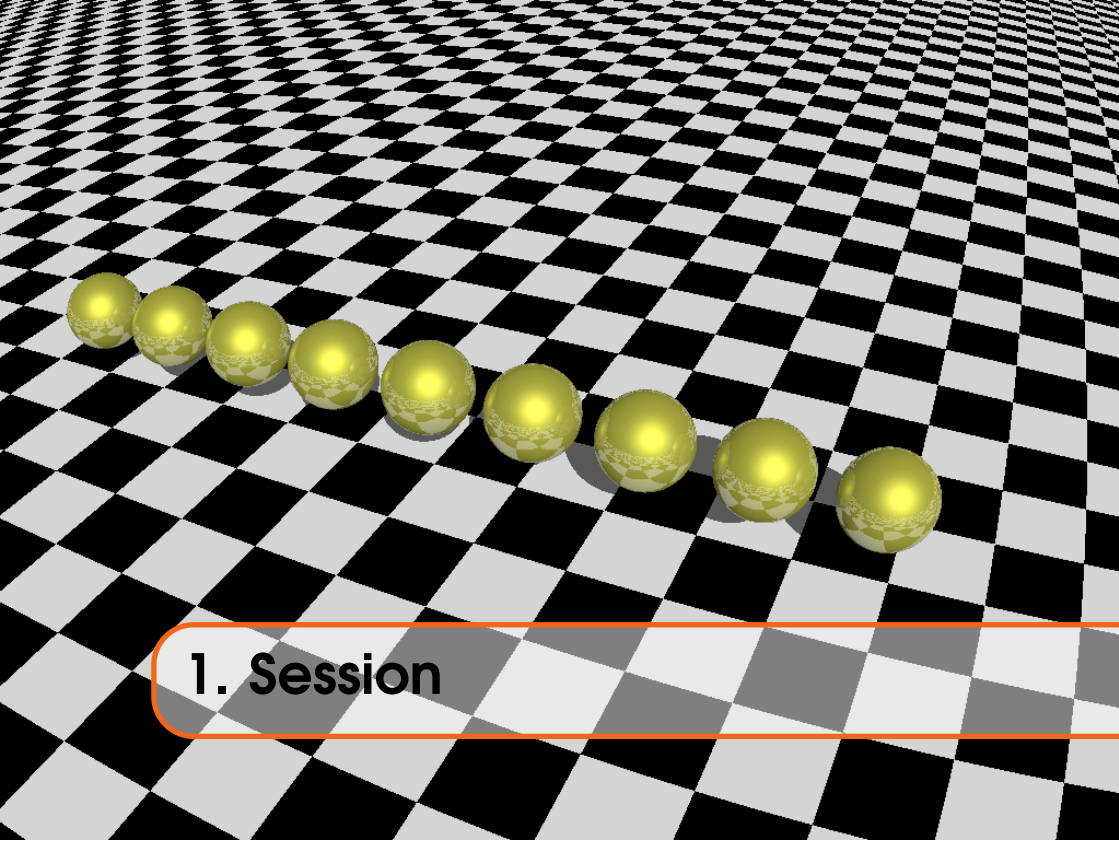
Vincenzo Giannini
Johannes Lischner
Arash Mostofi
John Pendry



Contents

III Fri 26th August

Wed 24th August



1. Session

12.30 - 13.30 **Lunch** & **Registration** *Room* **G05**

13.30 - 13.40 **Welcome** *Room* **G20**

13.40 - 14.15 Professor Jeremy Baumberg

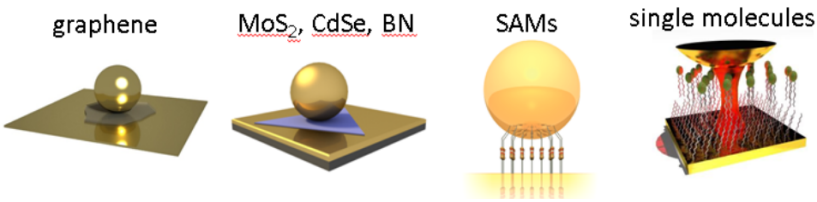
Room **G20: Single molecule plasmonics, strong coupling, and nanochemistry**

Abstract 1 — University of Cambridge. Coupling between plasmonic nano-components generates strongly red-shifted resonances combined with intense local field amplification on the nanoscale. This allows directly seeing molecules as well as excitations in semiconductors. We have recently

explored plasmonic coupling which can be tuned dynamically, through reliable bottom-up self-assembly. The crucial aspect of these systems is the extreme sensitivity to separation, and how quantum tunneling starts to be directly seen at room temperature in ambient conditions. We recently demonstrated how quantum plasmonics controls the very smallest space that light can be squeezed into.[1-3] Here we explore how quantum effects can play a role in such ultra-small cavities.

We also demonstrate the possibility to track few molecules using the extreme enhancements. We show how the new generation of 2D semiconductors can couple to such nano-scale gaps utilizes our nanoparticle on mirror geometry. We find that changing just a single atom on each molecule of a self-assembled monolayer can shift the plasmon by over 50nm, and produce surprising vibrational signatures.[4-8] These have encouraging prospective applications in (bio)molecular sensing as well as fundamental science.[9-15] We also now demonstrate strong coupling with single molecules in appropriately designed optical and molecular nano-structures. The ability to track and watch molecules interact and react opens up the ability to study chemistry molecule-by-molecule and potentially to control single reaction pathways.

1. *Nature* **491**, 574 (2012).
2. *ACS* Nano **5**, 3878 (2011).
3. *Nano Lett.* **13**, 5033 (2013).
4. *ACS Nano* **9**, 825 (2014).
5. *Nano Lett.* **15**, 669 (2015).
6. *Sci. Rep.* **4**, 5490 (2014).
7. *Nat. Comm.* **5**, 4568 (2014).
8. *Nat. Comm.* **5**, 3448 (2014).
9. *Sci. Rep.* **4**, 6785 (2014).
10. *Nano Lett.* **13**, 5985 (2013).
11. *Opt. Express* **23**, 33255 (2015).
12. *Nano Lett.* **15**, 2600 (2015).
13. *Phys. Rev.* **A 92**, 053811 (2015).
14. *Sci. Rep.* **5**, 16660 (2015).
15. *Nano Lett.* **15**, 7452 (2015).



16. *Nature in press* (2016).

14.15 - 14.50 Professor Ortwin Hess

Room **G20: Active Quantum Nanoplasmonics: From Single Quantum Emitter Strong Coupling to Stopped Light Nanolasing**

Abstract 2 — Imperial College of London. Recent progress in nanophotonics and metamaterials physics has prompted us to think of 'optics inside the wavelength' and exploit active nano-plasmonics and metamaterials as a new route to quantum many-body optics on the nanoscale [1,2]. At the same time, lasers have become smaller and smaller, reaching with the demonstration of plasmonic nanolasing, scales much smaller than the wavelength of the light they emit [3,4]. Such plasmonic nanolasers employ plasmonic resonances for feedback, allowing them to concentrate light into mode volumes that are no longer limited by diffraction.

The talk will discuss recent progress in the study of quantum emitters and quantum gain in nano-plasmonic cavities, combining classical and quantum many-body theory and simulation to describe and model the spatio-temporal dynamics of the optical near field and plasmon polaritons coupled with quantum emitters in nano-plasmonic cavities. Moreover, it will be demonstrated that applying the nanoplasmonic stopped-light lasing principle to surface- plasmon polaritons (SPP) allows the realization of trapped/condensed non-equilibrium surface-plasmon polaritons at stopped-light singularities, providing an entry point to SPP-condensation. We reveal

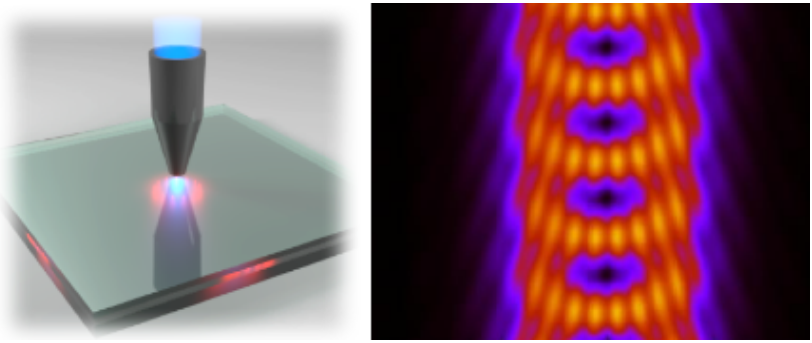


Figure 1.1: *Nano-lasing and surface plasmon polariton condensation at stopped-light singularities. Left: Lasing vortex in a nanoplasmonic waveguide. Right: Space (horizontal axis)- time (vertical axis) dynamics of active non-equilibrium surface-plasmon polaritons in a condensation.*

the mechanisms that experimentally (using plasmonic nanocavities scaled below 10 nm3 and host-guest chemistry to align 1-10 protectively-isolated quantum emitters) have recently allowed to reach the strong-coupling regime at room temperature and in ambient conditions [5].

1. *Nat. Mat.* **11**, 573 (2012).
2. *Science* **339**, 654 (2013).
3. *Nat. Comm.* **5**, 4971 (2014).
4. *Faraday Discuss* **178**, 307 (2015).
5. *Nat.* **535**, 127 (2016).

Coffee Break & Poster session

15.10 - 15.45 Professor Javier Aizpurua

Room **G20: Driving Plasmonics to the atomic scale**

Abstract 3 — Materials Physics Center (CSIC UPV/EHU) and DIPC. Plasmonic nanogaps are formed at the junction of two metallic interfaces and provide a great opportunity to explore atomic-scale morphologies and complex photochemical processes by optically monitoring the excitation of their intense surface plasmonic modes. In recent years, optical spectroscopy of these cavities has proven to be extremely sensitive to atomic-scale features that determine the chemistry and the optoelectronics in the gaps. In this

regime, classical theories often fail to address the fine details of the optical response, and more sophisticated quantum models are needed [1]. Indeed, quantum theoretical approaches can be properly developed to address the optics of extreme atomic-scale structures, such as in metallic nanogaps where the separation distances reach Ångstrom-scale dimensions. A few experimental situations in optoelectronics and molecular spectroscopy where optics is proven to address the atomic scale, and thus quantum effects are shown to be of paramount importance will be described in this talk.

1. *Nano Lett.* **15**, 3410 (2015).
2. *ACS Phot.* **3**, 269 (2016).
3. *Sci. Adv.* **1**, e1501095 (2015).

15.45 - 16.20 Professor Peter Nordlander

Room **G20: Quantum Plasmonics and hot carrier induced processes**

Abstract 4 — Rice University. Plasmon resonances with their dramatically enhanced cross sections for light harvesting have found numerous applications in a variety of applications such as single particle spectroscopies, chemical and biosensing, subwavelength waveguiding and optical devices.[1] Recently it has been demonstrated that quantum mechanical effects can have a pronounced influence on the physical properties of plasmons. Examples of such effects is the charge transfer plasmon enabled by conductive coupling (tunneling) between two nearby nanoparticles and nonlocal screening of the plasmonic response of small nanoparticles. One relatively recent discovery is that plasmons can serve as efficient generators of hot electrons and holes that can be harvested in applications. The physical mechanism for plasmon-induced hot carrier generation is plasmon decay. Plasmons can decay either radiatively or non-radiatively with a branching ratio that can be controlled by tuning the radiance of the plasmon mode. Non-radiative plasmon decay is a quantum mechanical process in

which one plasmon quantum is transferred to the conduction electrons of the nanostructure by excitation of an electron below the Fermi level of the metal into a state above the Fermi level but below the vacuum level. In particular I will discuss external control of charge transfer plasmons for active plasmonic devices,[2] molecular plasmonics,[3] hot carrier generation, decay and fluorescence,[4] and hot carrier induced processes and applications such as photodetection, photocatalysis, and phase changing of nearby media.[5]

1. *Adv. Mat.* 24, 4842 (2012), and *Acc. Chem. Res.* **45**, 1887 (2012).
2. *Sci. Adv.* **1**, e1500988 (2015); and ibid. e1501095.
3. *ACS Nano* **7** 3635 (2013) and *Nano Lett.* **15**, 6208 (2015).
4. *ACS Nano* **8**, 7630 (2014) and TBP(2016)
5. *Nat. Nanotech.* **10**, 25 (2015).

16.20 - 16.55 Professor Javier García de Abajo

Room **G20: Recent Advances in Graphene Nanophotonics**

Abstract 5 Recent experimental and theoretical advances in the study of graphene plasmons have triggered the search for similar phenomena in other materials that are structured down to the atomic scale, and in particular, alternative 2D crystals, noble-metal monolayers, and polycyclic aromatic hydrocarbons, which can be regarded as molecular versions of graphene. The number of valence electrons that are engaged in the plasmon excitations of these materials is small compared with those of conventional 3D metallic nanostructures, and consequently, the addition or removal of a comparatively small number of electrons produces sizeable changes in their frequencies and near-field distributions.

Graphene in particular has been shown to exhibit a large degree of electrical modulation due to its peculiar electronic band structure, which is characterized by a linear dispersion relation and vanishing of the electron

density of states at the Fermi level; few electrons are needed to considerably change the Fermi energy. However, plasmons in graphene have only been observed at mid-infrared and lower frequencies, and therefore, small molecular structures and atomically thin metals constitute attractive alternatives to achieve fast electro-optical modulation in the visible and near-infrared (vis-NIR) parts of the spectrum.

In this presentation, we review different strategies and recent advances in the achievement of strong optical tunability in the vis-NIR using plasmons of atomic-scale materials, as well as their potential application for quantum optics, light manipulation, and sensing.

16.55 - 17.30 Discussions

Thu 25th August

2. Session

09.15 - 09.30 Tea & Coffee *Room* G05

09.30 - 10.05 Professor N. Asger Mortensen

Room **G20: Nonlocal light-matter interactions in nanoscale plasmonics**

Abstract 6 — Technical University of Denmark. I will discuss ongoing experimental and theoretical efforts to explore the plasmonic response in metallic nanoparticles, where nanometric dimensions are expected to promote a nonlocal plasmonic response beyond that of the usual classical electrodynamics. In particular, efforts to make semi-classical hydrodynamic extensions [1,2] will be addressed, as well as developments beyond these

simplified models [3,4]. Experimentally, single-particle EELS has revealed nonlocal blueshifts of resonances in silver nanoparticles and nonlocal damping of high-order modes has been observed too [5]. I also discuss single-particle spectroscopy versus ensemble-averaged spectral properties, showing how Landau-related homogenous broadening dominates size-dependent inhomogeneous broadening [6]. Finally, I will discuss means to quantify the degree of nonclassical effects from an energy perspective [7].

1. *Nat. Comm.* **5**, 3809 (2014).
2. *J. Phys. Cond. Mat.* **27**, 183204 (2015).
3. *Nat. Comm.* **6**, 7132, (2015).
4. *Phys. Rev. Lett.* **115**, 137403 (2015).
5. *Nat. Comm.* **6**, 8788 (2015).
6. *Sci. Rep.* **6**, 28441 (2016).
7. *Phys. Rev.* **B 93**, 115439 (2006)

10.05 - 10.40 Professor Richard V. Craster

Room **G20: Singular asymptotics of surface-plasmon resonance**

Abstract 7 — Imperial College of London. Surface plasmons are collective electron-density oscillations at a metal-dielectric interface. In particular, localised surface-plasmon modes of nano-metallic structures with narrow non-metallic gaps, which enable a tuneable resonance frequency and a giant near-field enhancement, are at the heart of numerous nanophotonics applications. In this work, we elucidate the singular near-contact asymptotics of the plasmonic eigenvalue problem governing the resonant frequencies and modes of such structures. In the classical regime, valid for gap widths $>$ 1nm, we find a generic scaling describing the drastic redshift of the resonance frequency as the gap width is reduced, and in several prototypical dimer configurations derive explicit expressions for the plasmonic eigenvalues and eigenmodes using matched asymptotic expansions; we also derive expressions describing the resonant excitation of such modes by light based

on a weak-dissipation limit. In the sub-nanometric “nonlocal” regime, we show intuitively and by systematic analysis of the hydrodynamic Drude model that nonlocality manifests itself as a potential discontinuity, and in the near-contact limit equivalently as a widening of the gap. We thereby find the near-contact asymptotics as a renormalisation of the local asymptotics, and in particular a lower bound on plasmon frequency, scaling with the 1/4 power of the Fermi wavelength. Joint work with Vincenzo Giannini, Ory Schnitzer and Stefan A. Maier.

Coffee Break

11.00 - 11.35 Dr Antonio Fernández-Domínguez

Room **G20: Strong Coupling of a Single Quantum Emitter in a Plasmonic Gap Cavity**

Abstract 8 — Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid. In this talk, I will present a quasi-analytical transformation optics description of plasmon-exciton strong coupling at the single emitter level in the gap between two metal nanoparticles. This method allows for a thorough exploration of this hybrid system incorporating the full richness of its plasmonic spectrum. I will use this tool to solve the

Wigner-Weisskopf problem for this geometry, showing that by placing the emitter away from the cavity center, its coupling to multipolar dark modes of both even and odd parity increases remarkably. Finally, I will discuss the material and geometric conditions giving rise to reversible dynamics in the population of the quantum emitter for realistic implementations of this archetypal nanocavity.

11.35 - 12.10 Dr Prineha Narang

Room **G20: Generation, transport and relaxation dynamics of non-equilibrium carriers in quantum plasmonics**

Abstract 9 The dynamics of optically-excited electrons and holes at femtosecond time scales and nanometer length scales is critical in many applications including photovoltaics, photocatalysis and photodetectors. Decay of surface plasmons to hot carriers is a new direction that has attracted considerable fundamental and application interest, yet a theoretical understanding of ultrafast plasmon decay processes and the underlying microscopic mechanisms remain incomplete. While ultrafast experiments provide insights into the relaxation of non-equilibrium carriers at the tens and hundreds of femtoseconds time scales, they do not yet directly probe shorter times with nanometer spatial resolution. Theoretical calculations can access these scales and complement such experiments, but have so far been primarily restricted to free electron-like models.

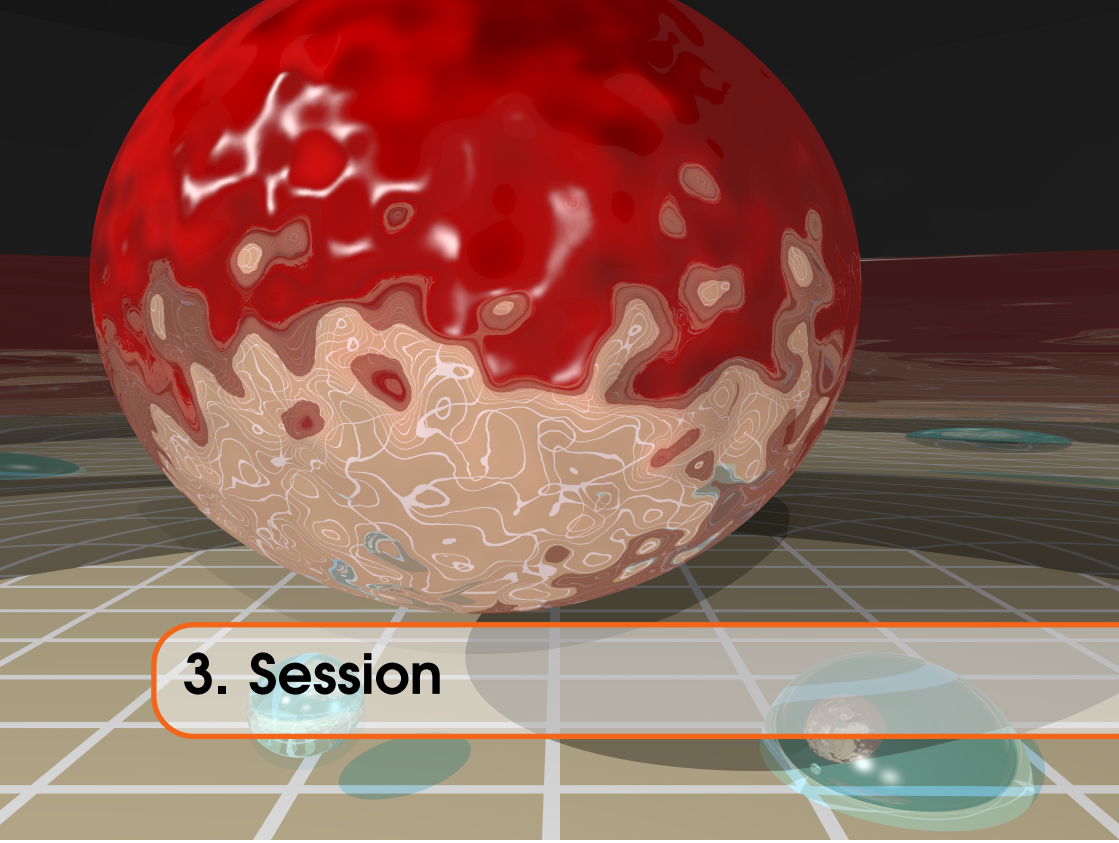
A theoretical understanding of plasmon-driven hot carrier generation and relaxation dynamics from the femtosecond to nanosecond timescales is presented here. We combine first principles calculations of electron-electron and electron-phonon scattering rates with Boltzmann transport simulations to predict the ultrafast dynamics and transport of carriers in real materials. In particular, we calculate the distributions of hot carriers generated by plasmon decay and their transport in metallic nanostructures which guide material selection and geometry design for plasmonic energy conversion devices. We also predict the evolution of electron distributions

in ultrafast experiments on noble metal nanoparticles from the femtosecond to picosecond time scales. In all these studies, we find that details in the electronic structure and electron-phonon coupling matter significantly, especially when *d* bands are involved.

The role of nonlinear multi-plasmon processes in measurements of plasmon decay has been suggested, yet the extent and spectral signatures of these contributions is an open question. Here we show calculations for multiplasmon and nonlinear processes in the ultrafast regime from the mid-IR to visible and in different geometries. Extending these predictions, we propose experimental signatures of the nonlinear response that utilize high-energy 'up-converted' carriers inaccessible from the linear response (conventional plasmon decay), including ultrafast measurements on metal-semiconductor interfaces and plasmon-enhanced Raman spectroscopy.

12.10 - 12.40 Discussions

Lunch & Poster session



3. Session

14.00 - 14.35 Dr Sterfano Corni

Room **G20: Characterizing plasmons and their interaction with molecules by first- principle simulations**

Abstract 10 — CNR Institute of Nanoscience. First principle methods such as time-dependent density functional theory are becoming increasingly popular in the investigation of surface plasmons localized on metallic nanoparticles and non-conventional plasmonic materials such as graphene nanoflakes. Besides revealing the dependence of the plasmon excitations on the microscopic details of the systems (atomistic geometry, role of surfactants and of the environment, etc.), such methods can also address basic questions such as the fundamental (quantum) nature of the plasmonic excitations themselves. In fact, nanoparticles and their excitations are composed

of electrons and nuclei like ordinary molecules. Therefore, it should be possible to understand their excited states, including plasmons, in terms of the same elementary electron-hole excitations routinely used to interpret molecular excited states, and to find the microscopic features that distinguish plasmonic from non-plasmonic excitations.

First principle methods are also useful to investigate the optical properties of molecules interacting with plasmonic nanosystems (e.g., to interpret surface-enhanced spectroscopies). Specifically, hybrid models can be devised for such systems, where the molecule is treated by a first principle method and the nanostructure as a continuous dielectric body. Such models can give access to the real-time optical behavior of the molecule plus plasmonic nanostructure system when interacting with short light pulses.

In this contribution I will discuss our on-going work to characterize the plasmonic nature of excitations by means of simple indexes that exploit the results of first-principle calculations [1]. I will also introduce some developments in hybrid models towards a real-time description of the molecule-metal nanoparticle systems [2].

1. *ACS Phot.* **1**, 1049 (2014) & *ACS Phot.* **3**, 520 (2016).
2. *J. Phys. Chem.* **A 119**, 5405 (2015).

14.35 - 15.10 Dr Tuomas Rossi

Room **G20: Quantized evolution of the plasmonic response in stretched nanorods**

Abstract 11 — Aalto University. Quantum aspects, such as electron tunneling between closely separated metallic nanoparticles, are crucial for understanding the plasmonic response of nanoscale systems. [1] In this work, we present, as a hitherto unrecognized fundamental quantum effect within the nanoplasmonics field, that the electronic structure restricting the charge flow plays a significant role in the plasmonic response. [2] To this aim, we consider adiabatic stretching of a metallic nanorod. This stretching process leads to the formation of a narrowing atomic contact between the

two nanorod ends until the rod splits into two. Based on first-principles time-dependent density-functional-theory calculations, we find that the response of the system goes through a series of discontinuous changes during the stretching. [2,3] This quantized evolution can be explained by the discrete nature of the electronic structure of the formed atomic-sized junction and can be considered as the plasmonic counterpart of the conductance quantization [4].

1. *Nat. Comm.* **7**, 11495 (2016).
2. *Phys. Rev. Lett.* **115**, 236804 (2015).
3. *ACS Phot.* **3**, 269 (2016).
4. *Phys. Rep.* **377**, 81 (2003).

Coffee Break & Poster Session

15.30 - 16.05 Professor Lucia Reining

Room **G20: Plasmons and electron-plasmon interaction: insight and predictions from ab initio approaches**

Abstract 12 — European Theoretical Spectroscopy Facility (ETSF). Plasmons are well understood as classical charge oscillations of the electron gas. They can be induced as direct reaction to external perturbations, or more indirectly, as a consequence of other excitations of the system. In real materials, where different groups of electrons can oscillate on different energy and length scales, the concept of a plasmon is less clear-cut. In order to describe plasmonic excitations and their couplingto other excitations in real systems, first-principles approaches that take into account the microscopic structure of materials, as well as many-body effects due to the

electronelectron interaction, have an important role to play. In this talk we will focus on the description and consequences of many-body effects.

We will discuss the calculation and understanding of plasmonic spectra, as well as the description and analysis of plasmon satellites in photoemission spectra. We will show ways to go beyond currently used approximations, and we will discuss fingerprints of correlation in photoemission and inelastic x-ray scattering spectra, making close connections between theory and experiment. Systems used for illustration will include models, simple metals and semiconductors, carbon nanostructures and transition metal oxides [2]. The results have been obtained in collaboration with many colleagues in the Theoretical Spectroscopy Group of the Laboratoire des Solides Irradiés and in the European Theoretical Spectroscopy Facility.

1. *Phys. Rev.* **139**, A796 (1965).
2. See e.g. *Phys. Rev. Lett.* **107**, 166401 (2011); *Phys. Rev.* **B 89**, 085425 (2014); *Phys. Rev. Lett.* **114**, 116402 (2015); *J. Chem. Phys.* **143**, 184109 (2015).

16.05 - 16.40 Professor Kristian Sommer Thygesen

Room **G20: Plasmonics with 2D materials**

Abstract 13 — Technical University of Denmark.

Two-dimensional (2D) materials such as graphene and monolayers of transition metal dichalcogenides have recently opened new possibilities for atomic-scale design of functional materials via stacking of different 2D crystals into van der Waals heterostructures.

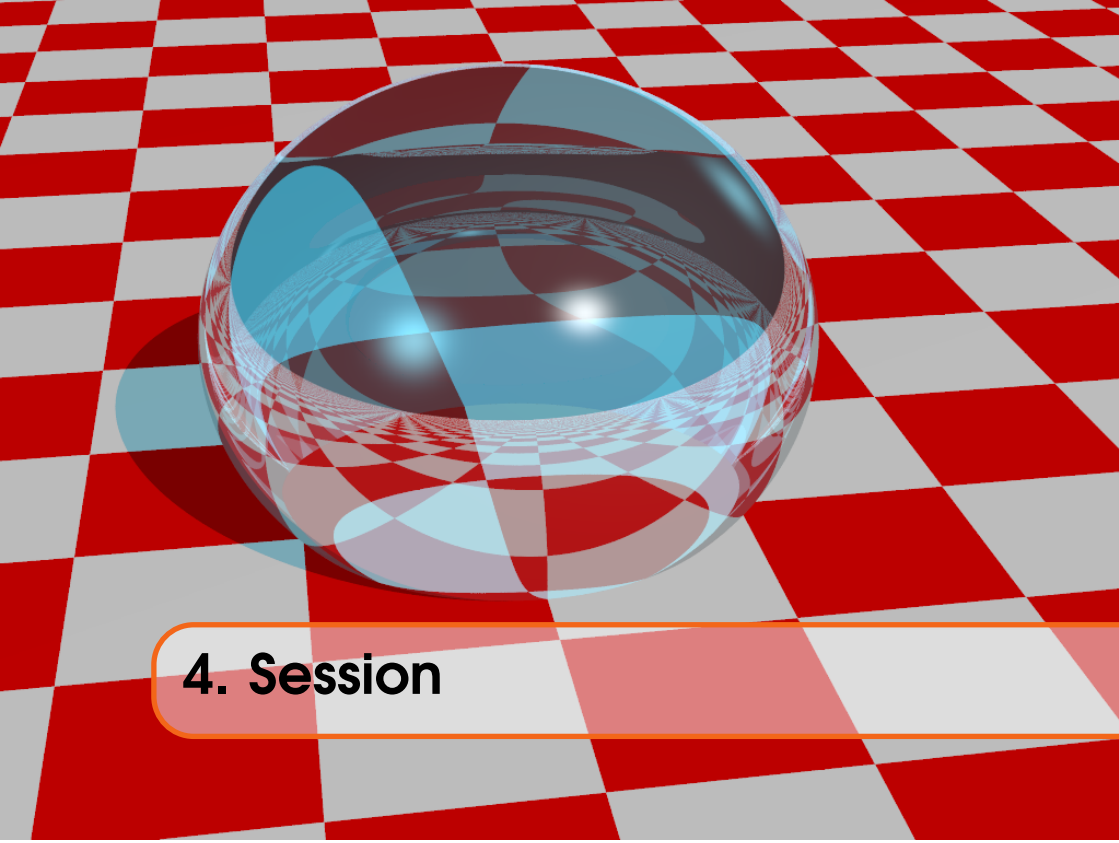
In the first part of this talk I will give a general introduction to the electronic structure of 2D materials, including the characteristic features of their dielectric function and collective excitations. I will show how the dielectric function of a given 2D material can be controlled by embedding it into a vdWH, and how this in turn can be used to design the band structure, exciton binding energies, or the plasmon energies in metallic layers.

In the second part I will show that layered van der Waals metals can exhibit unusually low optical losses in the mid-near infrared frequency regimes thanks to certain features of their metallic band structure which greatly suppresses the density of states for electron-hole scattering.

16.40 - 17.10 Discussions


18.30 Dinner

Fri 26th August



4. Session

09.15 - 09.30 Tea and Coffee *Room* G05

09.30 - 10.05 Professor Francisco J. García Vidal

Room G20: **Modifications Material and Chemical Properties of Organic Molecules Driven by QED Phenomena**

Abstract 14 — Condensed Matter Physics Center (IFIMAC) Universidad Autónoma de Madrid. Collective strong coupling of excitons with an electromagnetic (EM) confined mode is achieved when the energy exchange rate between exciton and EM field modes becomes faster than the decay rates of either constituent. In this talk we will show how some material and chemical properties of molecules can be tuned and modified by taking advantage of this QED phenomenon.

First we will show how exciton conductance in organic materials can be enhanced by several orders of magnitude when the molecules are strongly coupled to an EM confined mode. We demonstrate how the formation of collective strongly coupled modes (polaritons) allows excitons to bypass the disordered array of molecules [1]. Moreover, by designing the electric field profile of the EM mode that provides the strong coupling, transport properties can be tuned to achieve exciton harvesting and funneling [2]. As a byproduct of this research, we have also found that, surprisingly, the uncoupled dark states associated with the phenomenon of collective strong coupling can inherit the delocalized character of the polaritons [3], despite the fact that they do not have a photonic component.

Finally, we analyze under which conditions the molecular properties under strong coupling can be understood by the modification of the potential energy surfaces determining nuclear dynamics under the Born-Oppenheimer approximation [4]. In addition, we demonstrate that strong coupling of organic molecules to a confined light mode can be used to strongly suppress photoisomerization [5].

1. *Phys. Rev. Lett.* **114**, 196402 (2015).
2. *Phys. Rev.* **B 92**, 121402(R) (2015).
3. *arXiv* 1606.05513 (2016).
4. *Phys. Rev.* **X 5**, 041022 (2015).
5. *arXiv* 1606.04684 (2016).

10.05 - 10.40 Professor Ilya Tokatly

Room G20: Quantum Electrodynamical Time-Dependent Density Functional Theory

Abstract 15 — Universidad del País Vasco. In this talk I present a time-dependent density functional theory for many-electron systems strongly coupled to quantized electromagnetic modes of a microcavity (QED-TDDFT).

First I prove the basic mapping theorem stating that the electron- photon

wave function is a unique functional of the electronic density and the expectation values of photonic coordinates. Then, I introduce the Kohn-Sham construction that allows to calculate the above basic variables by solving self- consistent equations for a fictitious system of noninteracting particles.

Finally, I will discuss a practical approximation for the exchange-correlation functional in QED- TDDFT, which extends the concept of optimized effective potential (OEP) to electron-photon system.

1. *Phys. Rev. Lett.* **110**, 233001 (2013).
2. *Phys. Rev. Lett.* **115**, 093001 (2015).

10.40 - 11.15 Dr Cristian Ciracì

Room **G20: Current-dependent exchange-correlation potential for non-local absorption in quantum hydrodynamic theory**

Abstract 16 — Center for Biomolecular Nanotechnologies (CBN) Istituto Italiano di Tecnologia (IIT). A reliable description of optical properties of plasmonic nanostructures with different length scales requires methods beyond classical electromagnetism. A density functional approach allows a full description of the quantum nature of the free electrons however, it becomes prohibitive for clusters that exceed only few thousands atoms. An alternative approach is to use the hydrodynamic model that takes into account the nonlocal behavior of the electron response by including the electron pressure and can be generalized in order to describe spill-out effects near metal surfaces.

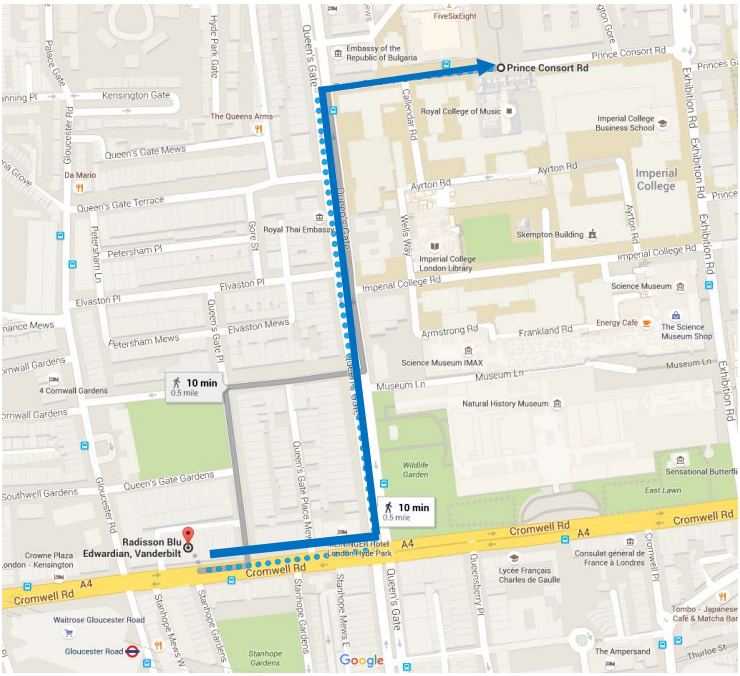
We show that the hydrodynamic model can be derived from the single particle Kohn-Sham equation and include the contribution of an external vector potential. This derivation allows to straightforwardly incorporate in the hydrodynamic description an exchange-correlation viscoelastic term, so that broadening of collective excitation can be taken into account, as well as a correction to the plasmon dispersion.

The result is an accurate self-consistent and computationally efficient description that is in great agreement with TDDFT calculations. Differently from DFT techniques however, the present model can be applied to structures containing tens of millions of electrons.

11.15 - 11.30 Coffee Break

11.30 - 12.00 Discussions

Location and Map



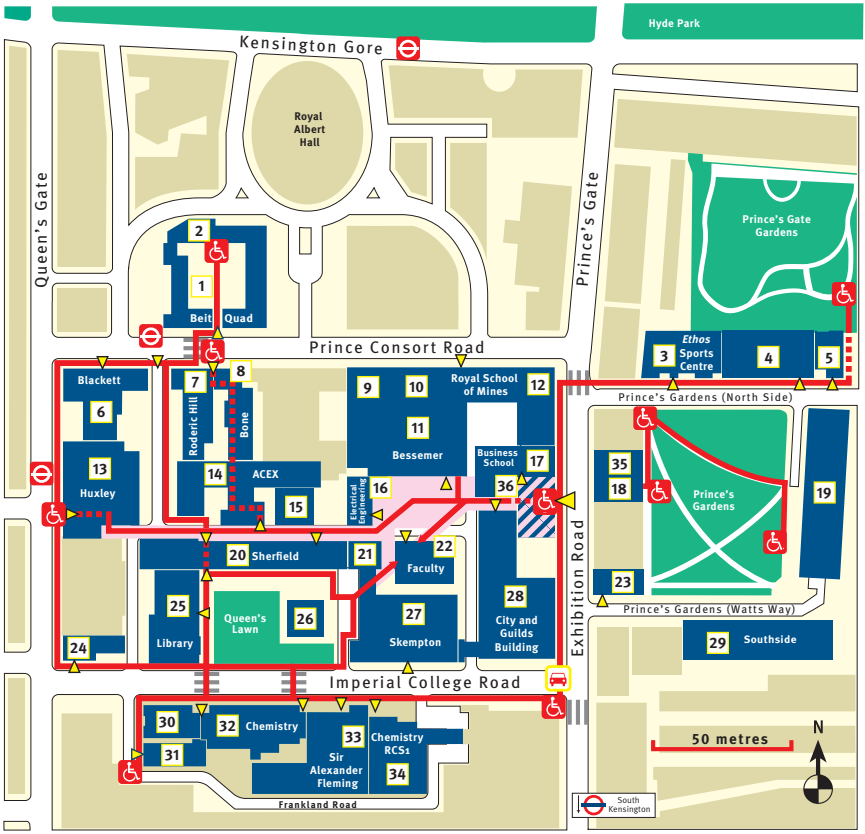
Accommodation:

Radisson Blu Edwardian Vanderbilt Hotel
68-86 Cromwell Road
Kensington
London, SW7 5BT
United Kingdom

Workshop Venue:
Lecture Room G20
Royal School of Mines
Imperial College London
Prince Consort Road
South Kensington Campus
London, SW7 2AZ

Imperial College London

South Kensington Campus



Main walkway

Main entrance

Accessible route

Buildings where wheelchair access is not possible at this time

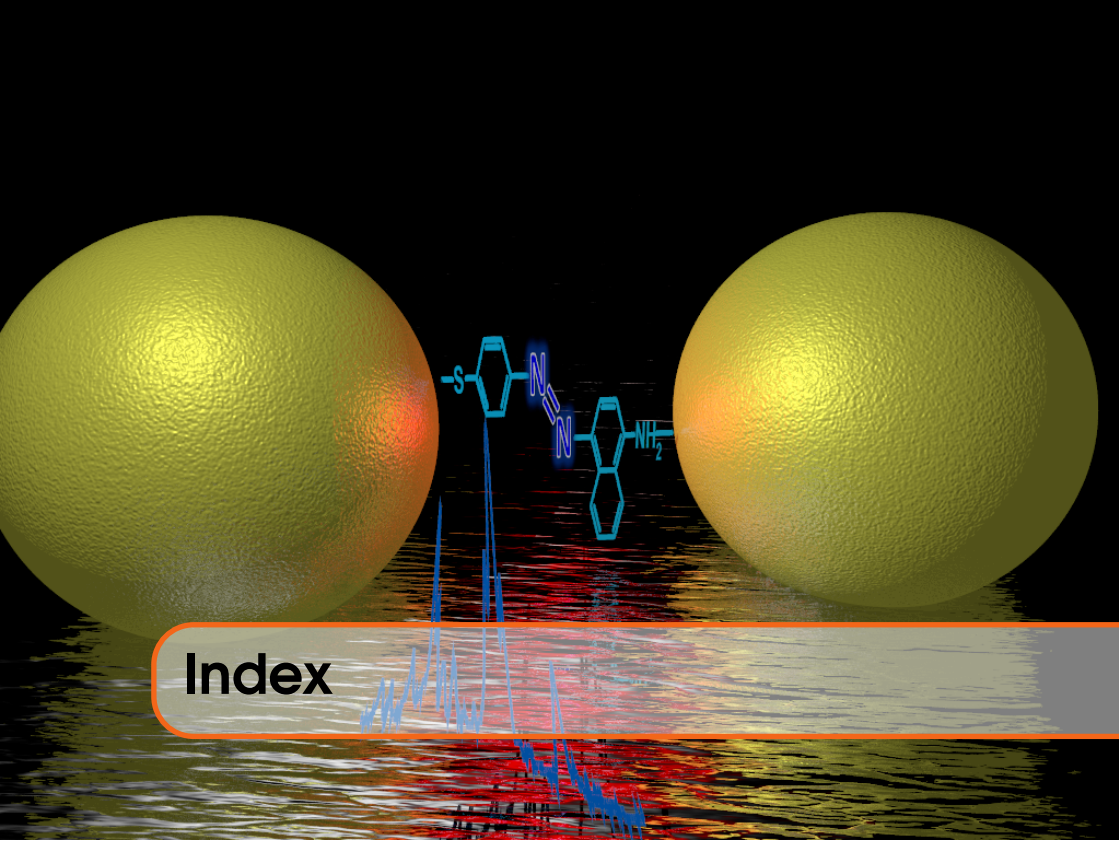
South Kensington Underground

Bus stops

Building entrances

Vehicle entrance

1	Beit Quadrangle
2	Imperial College Union
3	*Ethos* Sports Centre
4	Prince's Gdns, North Side
5	Weeks Hall
6	Blackett Laboratory
7	Roderic Hill Building
8	Bone Building
9	Royal School of Mines
10	Aston Webb
11	Bessemer Building
12	Goldsmiths Building
13	Huxley Building
14	ACE Extension
15	William Penney Laboratory
16	Electrical Engineering
17	Business School
18	53 Prince's Gate
19	Eastside
20	Sherfield Building Student Hub Conference Office
21	Grantham Institute for Climate Change
22	Faculty Building
23	58 Prince's Gate
24	170 Queen's Gate
25	Central Library
26	Queen's Tower
27	Skempton Building
28	City and Guilds Building
29	Southside
30	Sir Ernst Chain Building – Wolfson Laboratories
31	Flowers Building
32	Chemistry Building
33	Sir Alexander Fleming Building
34	Chemistry RCS1
35	52 Prince's Gate
36	Alumni Visitor Centre



Index

cecam

Centre Européen de Calcul Atomique et Moléculaire

EPSRC

IOP

Institute of Physics

Imperial College London

QUPLA