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Presentation of the L_Sim laboratory

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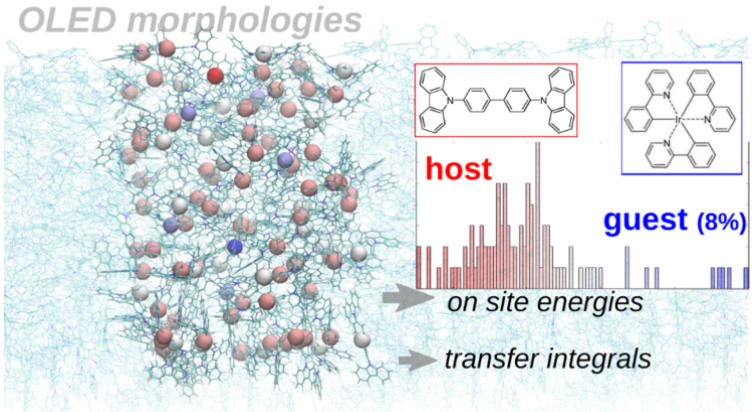
Interdisciplinary Research Institute of Grenoble (IRIG)

Service “Modeling and Exploration of Materials” (MEM)

Laboratory of atomistic simulation (L_Sim)

Presentation of the laboratory

- *L_Sim* is modeling the structural and electronic properties of materials and nanostructures down to the atomic scale using a wide variety of analytical techniques and numerical simulation tools:
  - ***Ab initio* density functional theory (DFT)**.
    DFT aims at predicting the ground-state properties of materials and nanostructures from « first-principles » (treating the atomic potentials « exactly » and making some suitable approximation for the Coulomb interactions).

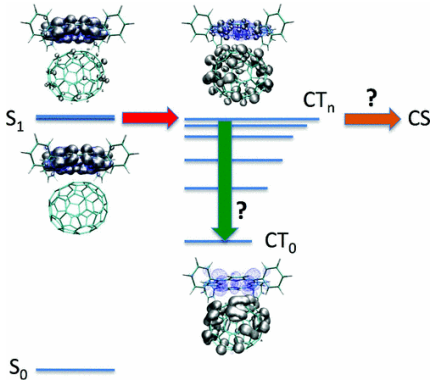


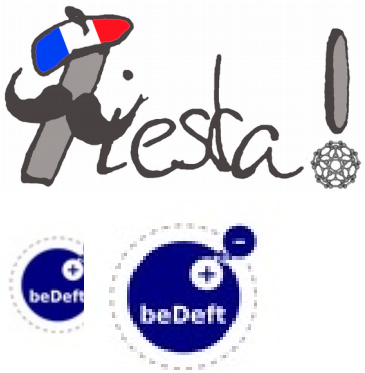
L_Sim is, in particular, developping « **BigDFT** », a DFT code using wavelets for large scale systems (up to many thousands atoms ~50k).

Presentation of the laboratory

- *L_Sim* is modeling the structural and electronic properties of materials and nanostructures down to the atomic scale using a wide variety of analytical techniques and numerical simulation tools:

  - **Many-body *GW* and TDDFT**.
    These methods aim at computing the electronic excitations and dynamics of the systems from first principles, using again various approximations for the Coulomb interactions.

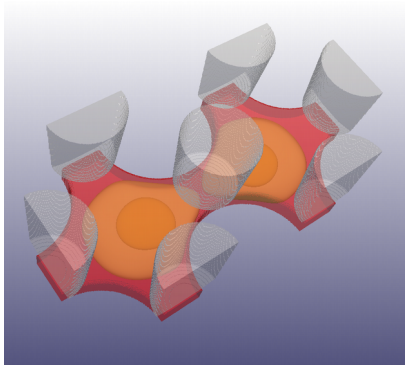


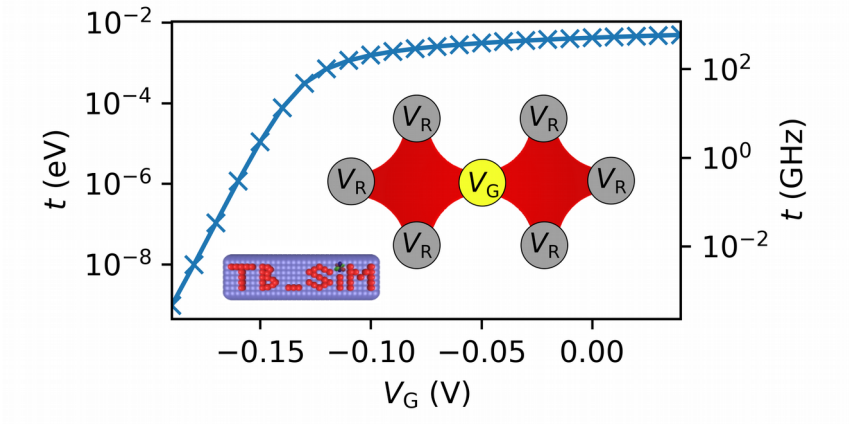


L_Sim is developing the « **Fiesta** » (now beDeft) code for the calculation of *GW* excitations in atomic orbitals-like basis sets.

Presentation of the laboratory

- *L_Sim* is modeling the structural and electronic properties of materials and nanostructures down to the atomic scale using a wide variety of analytical techniques and numerical simulation tools:
  - **k.p (effective mass) and tight-binding methods.**
    These methods aim at describing very large systems with millions of atoms, making suitable (but reasonable) approximations on both the atomic potentials and Coulomb interactions.





L_Sim is developing the « **TB_Sim** » code for the modeling of the electronic, optical and transport properties of semiconductor nanostructures.

Presentation of the laboratory

- Numerical simulation is an important part of the activity of the L_Sim laboratory
- For that purpose, L_Sim has access to large scale high-performance computing infrastructures, at the local, national and european levels :

- L_Sim = 7 permanent researchers + ~ 10 PhD students and postdocs.

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Modeling coherent operations on spin qubit arrays

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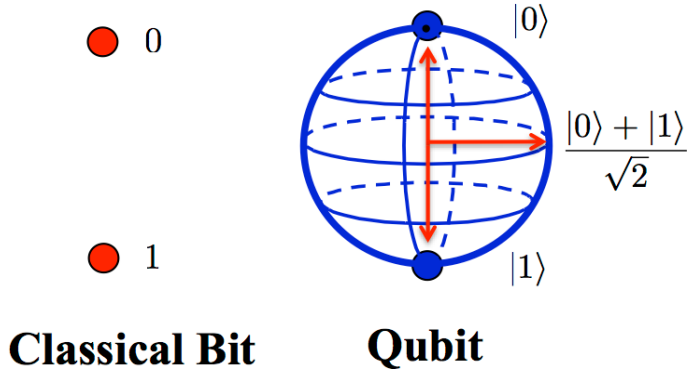


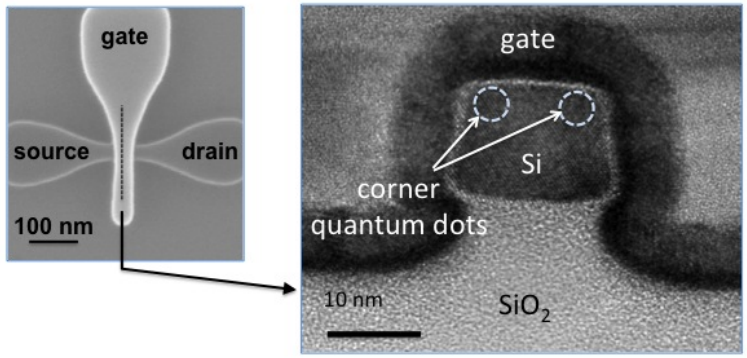
Quantum bit: Store information as a **coherent superposition** of « $|0\rangle$ » and « $|1\rangle$ » states

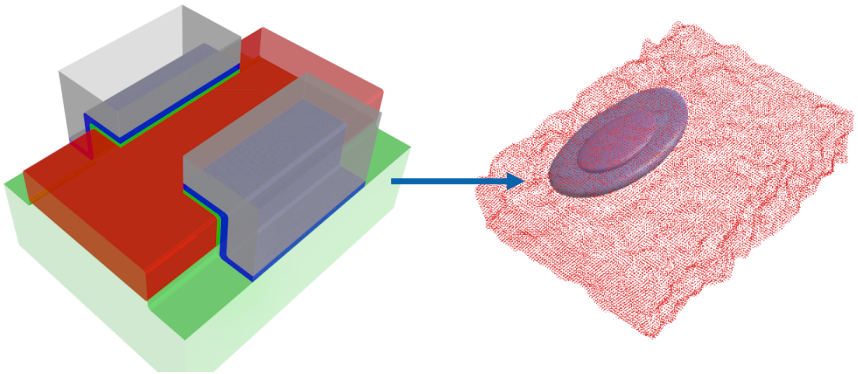
Benefits: Exponential speed-up with respect to classical information for some problems

Possible implementation: $|0\rangle \equiv |\downarrow\rangle$, $|1\rangle \equiv |\uparrow\rangle$ states of an electron in a « **single electron transistor** »

The spin is manipulated with RF pulses on the gates

Quantum computation: Entanglement by exchange (Coulomb+tunnel) interactions between qubits

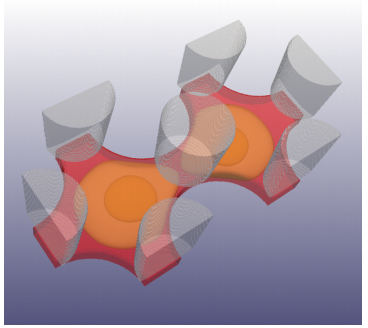




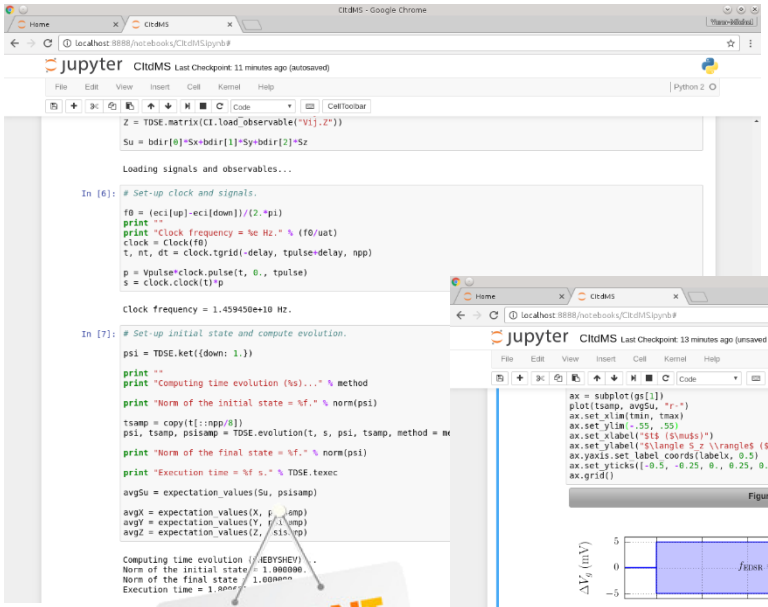
Strong need for modeling:
Quantum confinement and Coulomb correlations, manipulation based on spin-orbit coupling, decoherence....

Objective: **Modeling coherent operations on spin qubit arrays.**

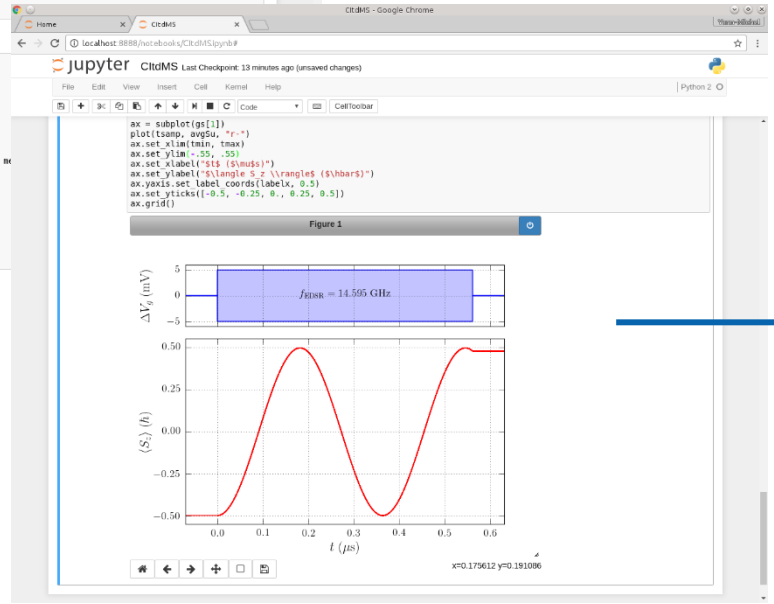
Framework: Electronic structure calculations on realistic geometries.
Interactive Python scripts for time-dependent simulations.
Analytical, effective models for interacting qubits.



TB_SiM



$$f_R^{(2)} = \frac{2^8 m_0 e^3}{3^4 \pi^9 \hbar^4} B|E_0|E_{ac} \frac{\gamma_3|\kappa|}{\gamma_2(\gamma_1+\gamma_2)^2} L_y^6 \frac{L_z^2}{L_y^2} G(\theta)\sin\theta$$



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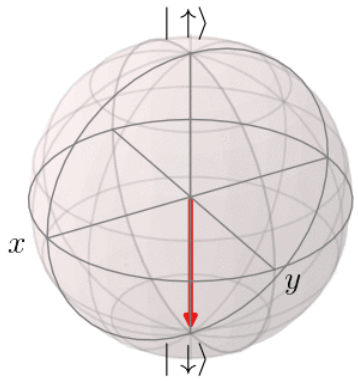
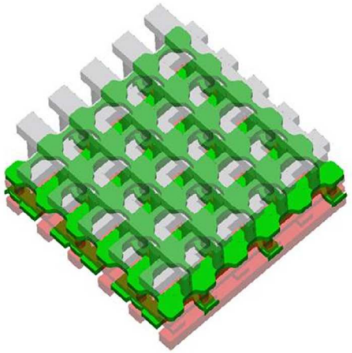
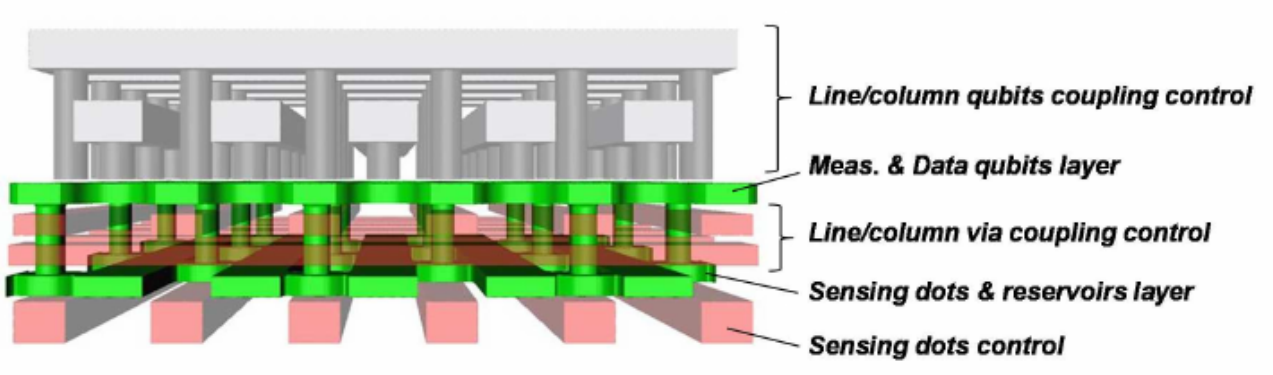
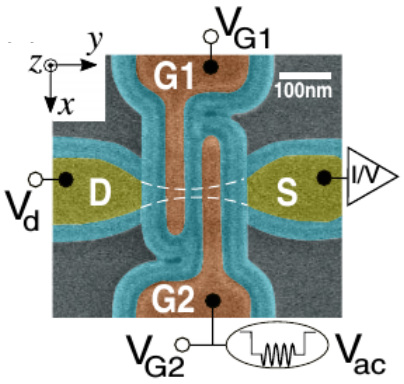


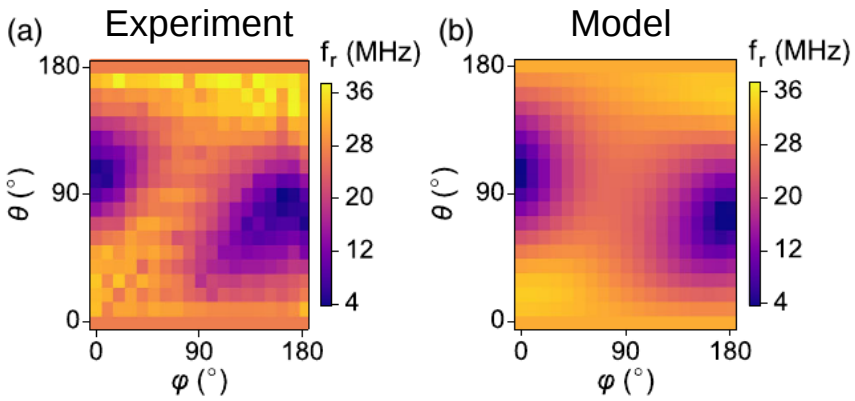
Context: **ERC Synergy "quCube" (2019-2024) gathering CEA/LETI, CEA/INAC and CNRS/Néel around the realization of 2D arrays of qubits (budget: 14 M€).**





Strong connections with experimental teams at CEA and in Europe (many joint publications since 2018).





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Hybrid simulation of III-V & II-VI semiconductor surfaces

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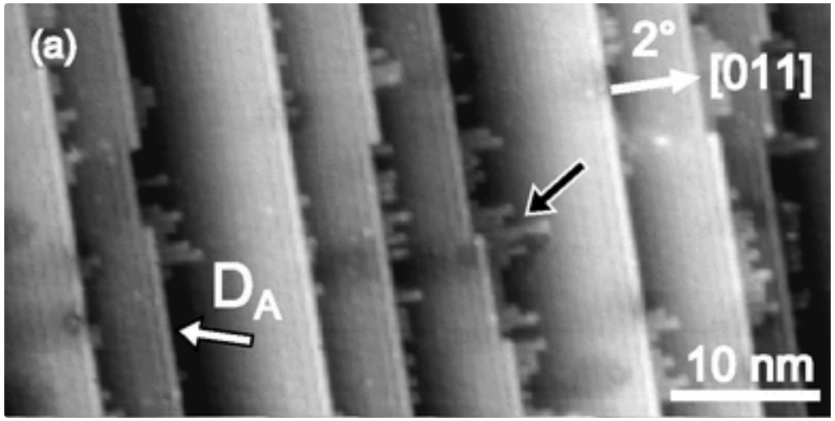
Pascal Pochet (pascal.pochet@cea.fr)

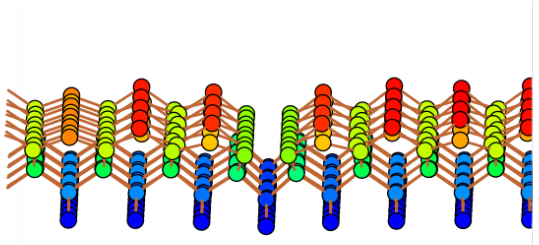
Context: **Surface science / 2D materials**

Defects, ad-atoms, surface reconstructions… require precise electronic modelling using *ab initio* methods. But also induce long range elastic deformations not tractable within usual DFT super-cells

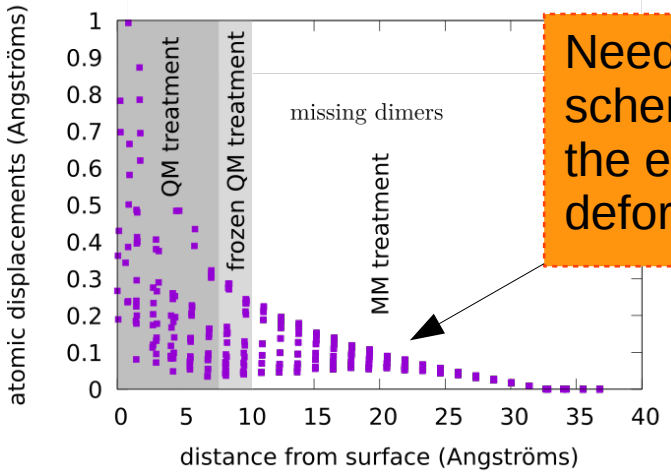
Example of hydrogen etched Si (001) surface for co-integration of III-V materials



The selective removal of silicon dimers on the surface is assisted by hydrogen, creating a miscut making the growth of III-V materials on top free of anti-phase boundaries.



DFT slab of a missing line of dimers



Need for a hybrid scheme to treat the elastic deformation tail

« Toward the III–V/Si co-integration by controlling the biatomic steps on hydrogenated Si (001) » Appl. Phys. Lett. 109 25 253103 (2016)

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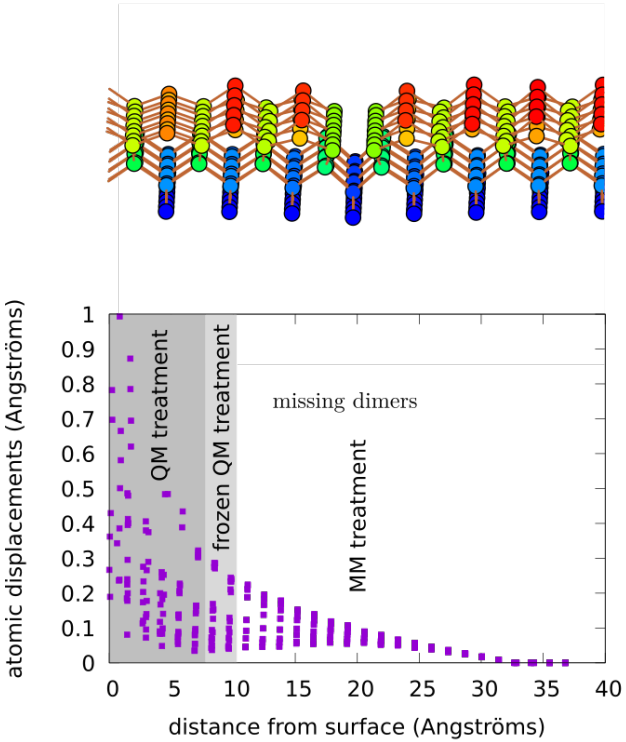

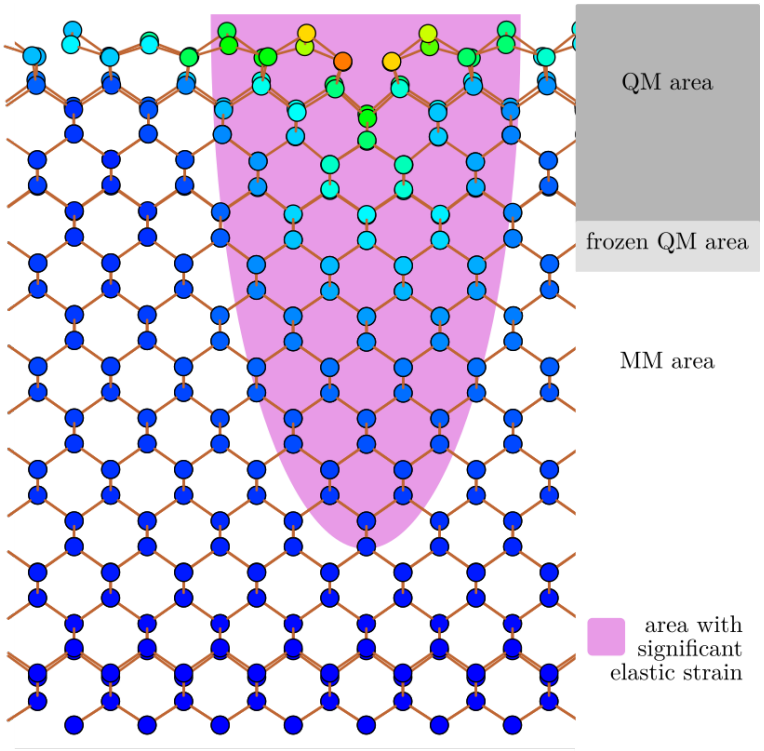

Quantum treatment on wavelet basis-set

Force-fields, added in a QM/MM approach

Subject: **The goal of the master thesis is to enhance the catalog of available force fields for III-V and II-VI. The developed method will be applied on a system connected to quantum computing material for which STM topographies are available from our experimental partners.**

A PhD grant is available to continue working on QM/MM simulations in relation to STM images of interfaces for growth over MoS_2 and SiC

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Revisitation de Formalismes de Réponse Linéaires basés sur la DFT

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Contexte: l'approche Time-Dependent Density Functional Theory (TDDFT) est un outil qui s'est établi dans la communauté comme une référence, utilisé comme base pour la mise à point de méthodes plus précis comme par exemple le formalisme de Bethe-Salpeter de la théorie de perturbation à multi-corps.

On propose deux sujets au croisement entre mathématiques appliquées et chimie computationnelle:

A) Le role de la causalité des intéractions dans le formalisme TDDFT

La description actuelle de la TDDFT assume que le potentiel d'intéraction entre deux électrons est instantané. On propose de **revisiter le formalisme TDDFT** dans l'hypothèse d'une intéraction non-instantanée, afin de vérifier le **rôle de la causalité** dans les différents termes qui contribuent au couplage entre excitations du système. Ainsi, il sera possible de fournir une base potentiellement justifiée sur laquelle il sera très facile de développer des théories de perturbations à multi-corps.

B) Discrétisation du spectre continu et application au calcul de spectres de photoabsorption

Dans le cas des sytèmes moléculaires, les propriétés d'ionisation de molécules et de réponse des solides impliquent un **continuum d'états** de diffusion ou de conduction, qui sont délocalisés. Les calculs numériques travaillent nécessairement dans un domaine de calcul de taille finie, ce qui a pour effet de **discrétiser et de localiser** ces états. En conséquence, l'approximation de fonctions de réponse nécessite une régularisation et converge lentement avec la taille du domaine de calcul.

L'objectif du stage est d'éclairer ce problème et d'explorer quelques pistes de résolution. Après une revue bibliographique du domaine, le candidat étudiera ce phénomène concrètement sur des **modèles simples** (type modèles de liaisons fortes), ainsi que quelques pistes de résolution (régularisation adaptative, complex scaling, conditions aux limites absorbantes, fonctions de Green, bases d'états résonants...) En fonction de l'avancement, une étude de modèles plus complexes (TDDFT) pourra être envisagée.

Profil: mathématiques appliquées, physique de la matière condensée, chimie théorique ou équivalent est attendu. Ce stage est **fortement multidisciplinaire**, et nécessite des compétences et un goût à la fois pour les aspects physiques et mathématiques.