Youth Workshop Collaboration - Nonlinear Eigenvalue Problems in Electronic Structure Calculations

~Collaborations on computational science and computer science~

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Target: Modeling Electronic Transport

- Our goal is to model electron transport from first principles in a variety of systems.
- Examples
  - 2 Dimensional Electronic Gas
  - Quantum dot
  - Solar Cell
  - Water Splitting
- Modeling electron transport requires new methods to be integrated into standard electronic structure software packages.

Background: Our Mutual Interests

- Study of solid state systems and their properties from first principles.
- The interest is not just in the ground state structure, but also excited state properties
- Frequently these studies require solving some type of eigenvalue problem.

Nonlinear eigenvalue problem

- M(λ)x=0, $M(\lambda) = \sum_{i=0}^{\infty} M_i \frac{\lambda^i}{i!}$
- Size of M_i is more than a few hundreds
- Compute (λ,x)
- Examples

  Flow of electric current

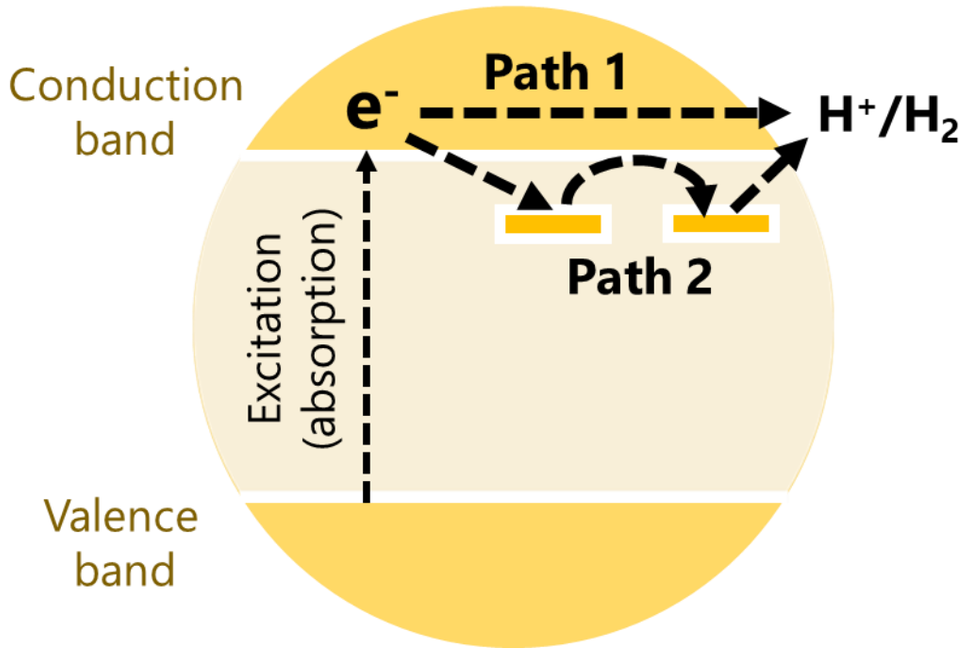
  Stability of flow

  Quantum mechanics

Transport of excited carrier in semiconductor photocatalyst

- Solar light absorption ~50%
- Reaction efficiency **~1%**

-> Enhancing the carrier transport is important



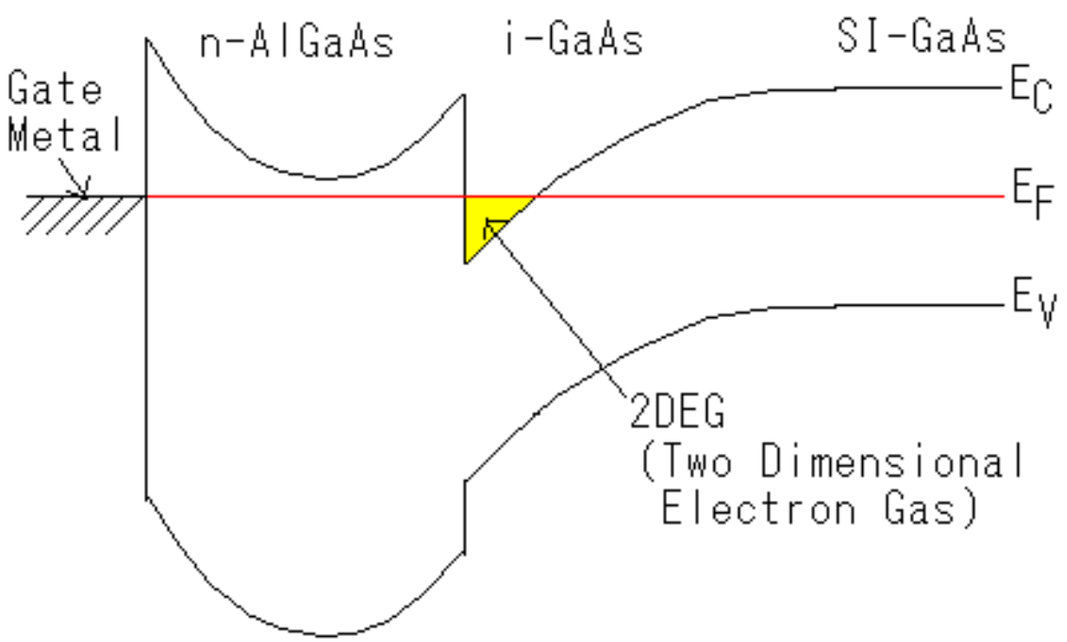
- Two possible path of excited carrier transport.

1. Carriers propagating in conduction bands.

2. Carriers hopping between defect levels.

-> Identify the dominant one by estimating the time scale of both paths.

Two Dimensional Electron Gas (2DEG)



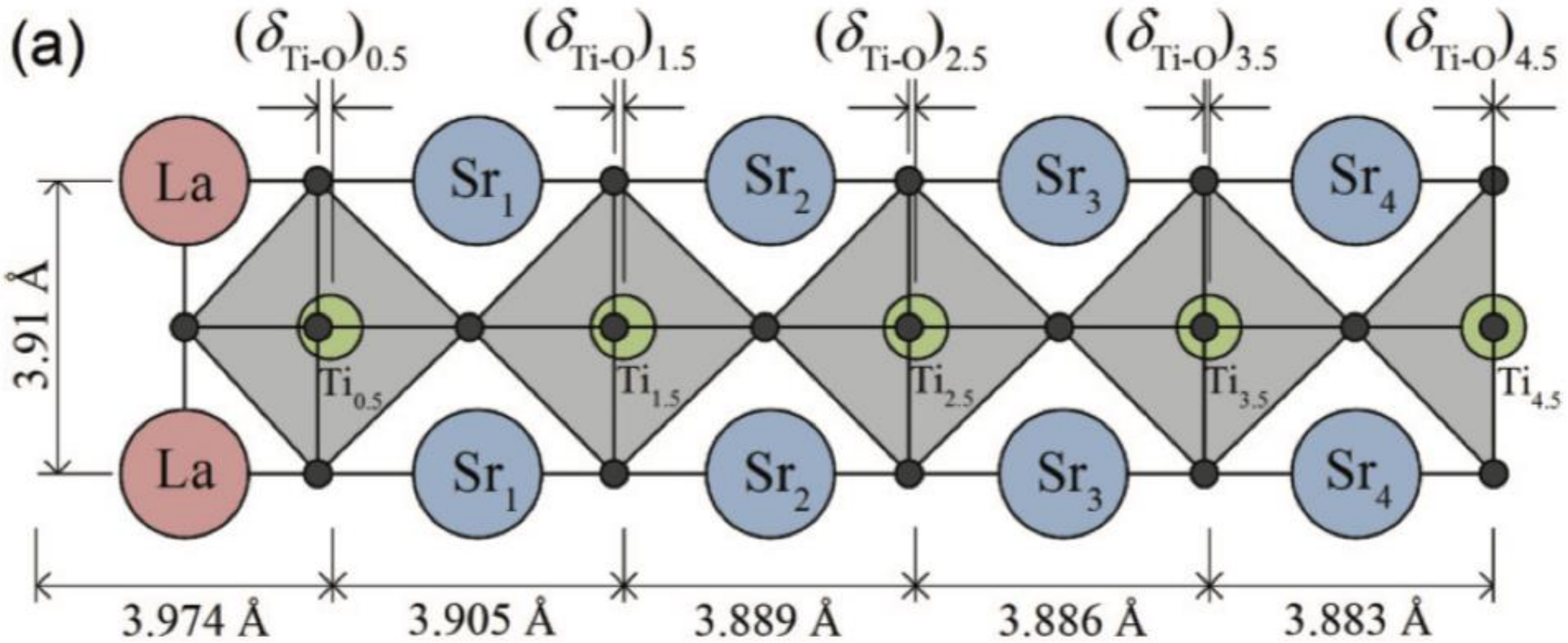
(https://en.wikipedia.org/wiki/Two-dimensional_electron_gas)

Electrons get trapped as the surface of the heterostructure due to the band bending.

They are free to move in 2D but confined in the third, that lead to quantized energy levels for the motion in the third direction

This system of electrons is of particular interest to scientist because of its high mobility in the two dimensions in which the electrons are free as it is comparable or even higher than in most metals

Critical thickness for the two-dimensional electron gas in $LaTiO_3/SrTiO_3$ superlattices



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Challenge

Superlattice calculations for modeling the heterojunction

Bigger superlattice for modeling system of heterojunction with defects

Bigger bigger superlattice for modeling system of heterojunction with defect that can created 2DEG

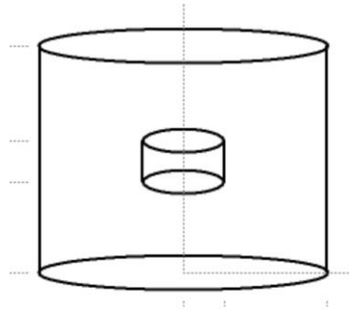
NEP - Electronic Calculations

- DFT: essential tool for studying the quantum mechanical properties of molecules, solids and other nanoscale materials
- Reduction of the many-body Schroedinger equation to a set of non-interacting-particle Kohn-Sham equations
- Price to pay ⟶ Nonlinear eigenvalue problem
- The Hamiltonian is a function of the desired but unknown eigenfunctions to be computed

NEP - Quantum Nanostructures

- Devices where the motion of charge carriers are confined
  - Quantum well (2D), Quantum wires (1D), Quantum dots (0D)
- Schroedinger equation of a Quantum Dot:

$$-\nabla\left(\frac{\hbar}{2m}\nabla\psi\right) + V\psi = \lambda\psi$$



- At the interface, *m* and *V* are discontinuous and in some models the effective mass is dependent on the eigenvalues

Krylov subspace method (iterative method)

$$M(\lambda) = \sum_{i=0}^{\infty} M_i \frac{\lambda^i}{i!}$$

- Algorithm

1 compute $B_{i-1} = -\frac{1}{i} M_0^{-1} M_i \ (i \geq 1)$

for $j = 1$ to $j = N$

2 Vector x is a eigenvector of the iteration before

$$\begin{cases} [y_1 \cdots y_N] = \left[\frac{x_0}{1} \cdots \frac{x_{N-1}}{N}\right] \\ y_0 = \sum_{i=0}^{N-1} B_i x_i \end{cases}$$

3 Gram-Schmidt orthogonalization on vector y

4 compute (λ,x) and do convergence judgment

Parallelization

- Algorithm

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Matrix vector parallelization

Well known parallelization

3 Gram-Schmidt orthogonalization on vector y

4 compute (λ,x) and do convergence judgment

Conclusion

- Our goal is to model electron transport from first principles in a variety of systems
- Examples of apps have been shown:
  - Transport of excited carrier in semiconductor photocatalyst
    - 2DEG
    - Quantum dot
    - DFT
- Effective eigen solver has been proposed
- Parallelization has been discussed