Application of Compressed Sensing to Quantum Chemistry

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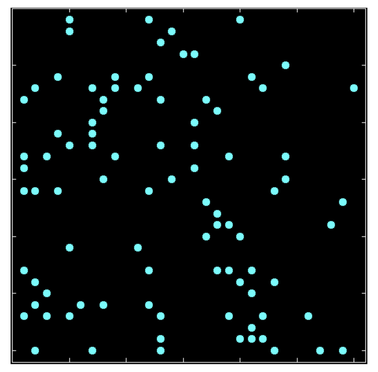
(A) Research Objective:

Use compressed sensing to calculate quantum chemistry matrices (Hamiltonian, Fockian, etc) cheaply without having to compute each matrix element.

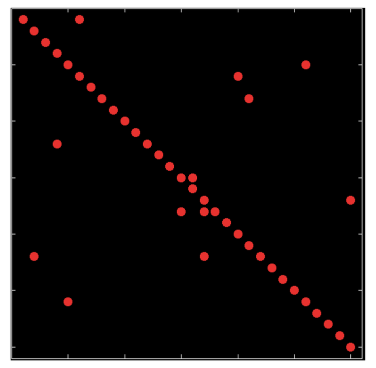
(B) Recovering a Matrix with Compressed Sensing

- **Step1**: Cheaply locate a basis in which the matrix is **sparse**.

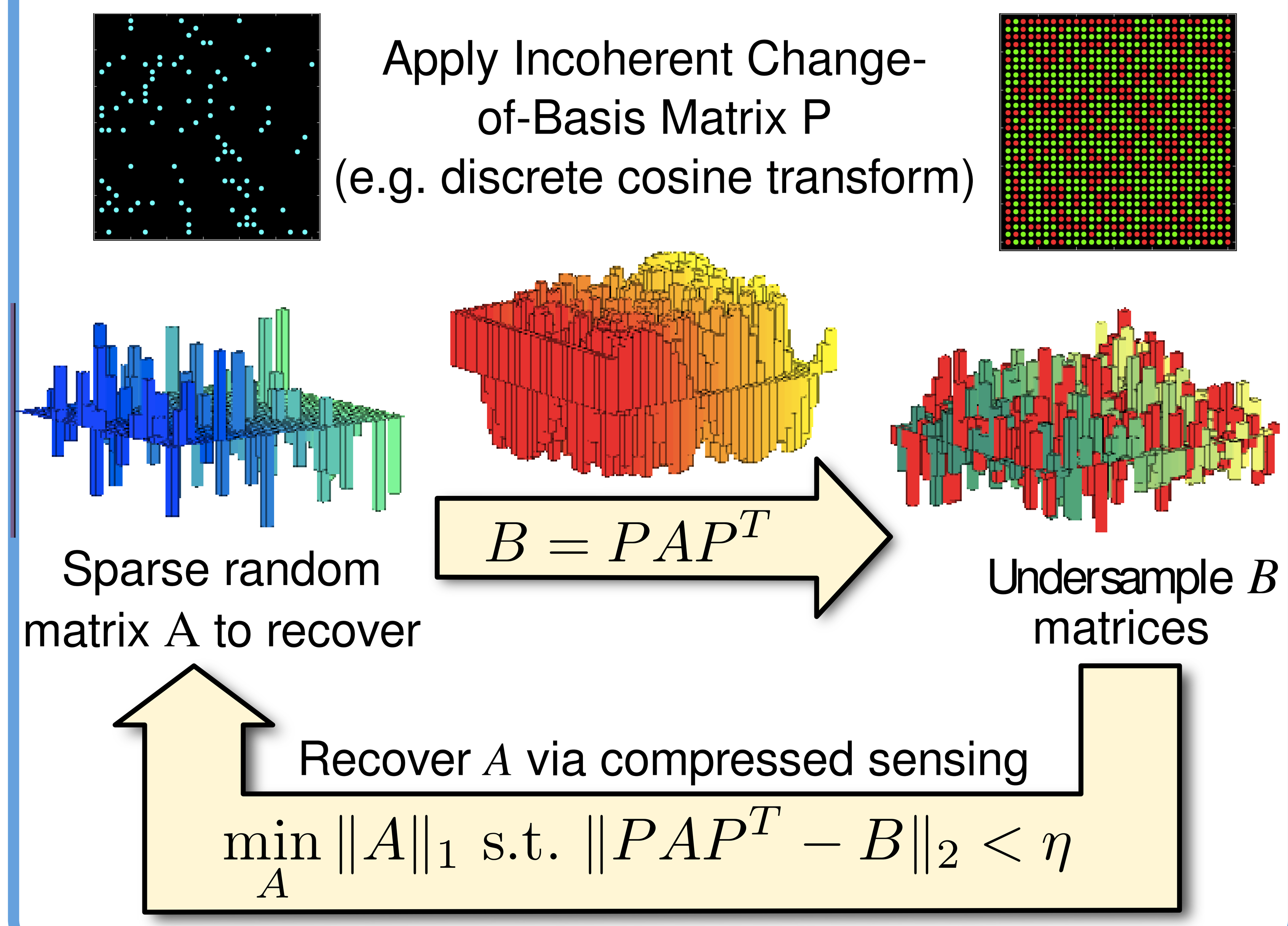
  Example: cheaply approximate the **eigenvectors.**



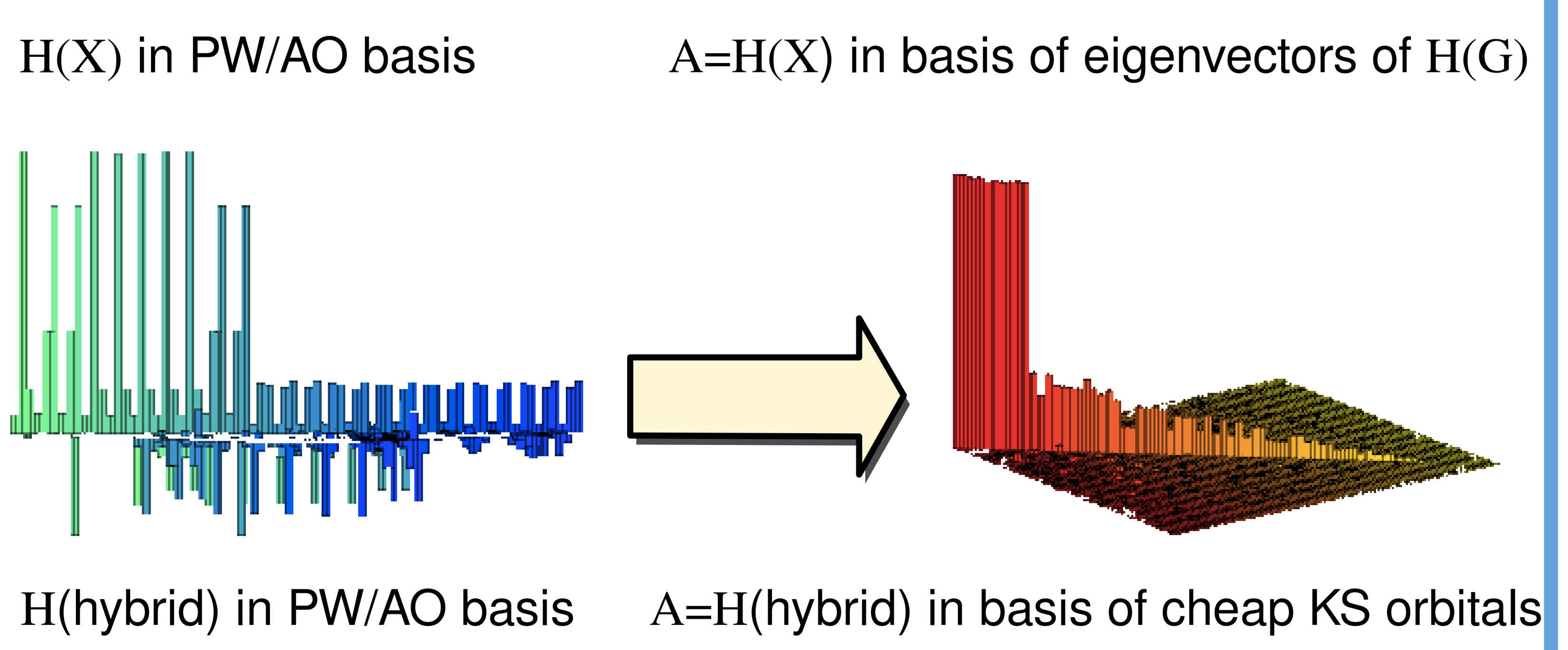
- **Step 2**: Cheaply recover this sparse matrix using compressed sensing.



(C) Compressed Sensing for Sparse Matrices



(D) Approach for Electronic Structure Calculations



A is a sparse matrix that can be recovered with our procedure.

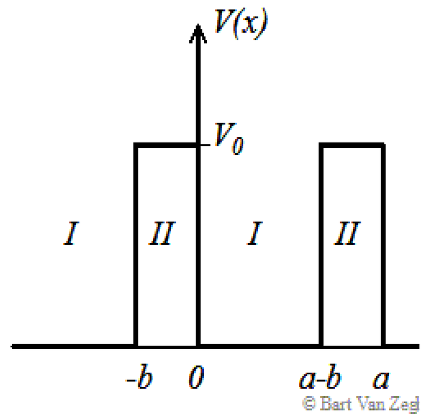
(E) The Kronig-Penney model

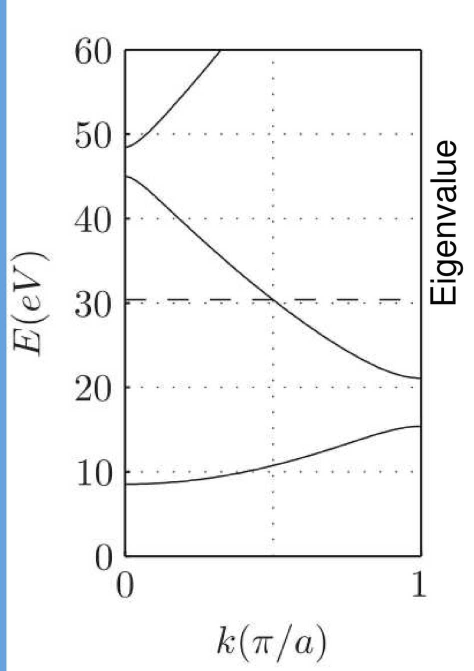
Physica B **406**, *4373-4380* (2011)

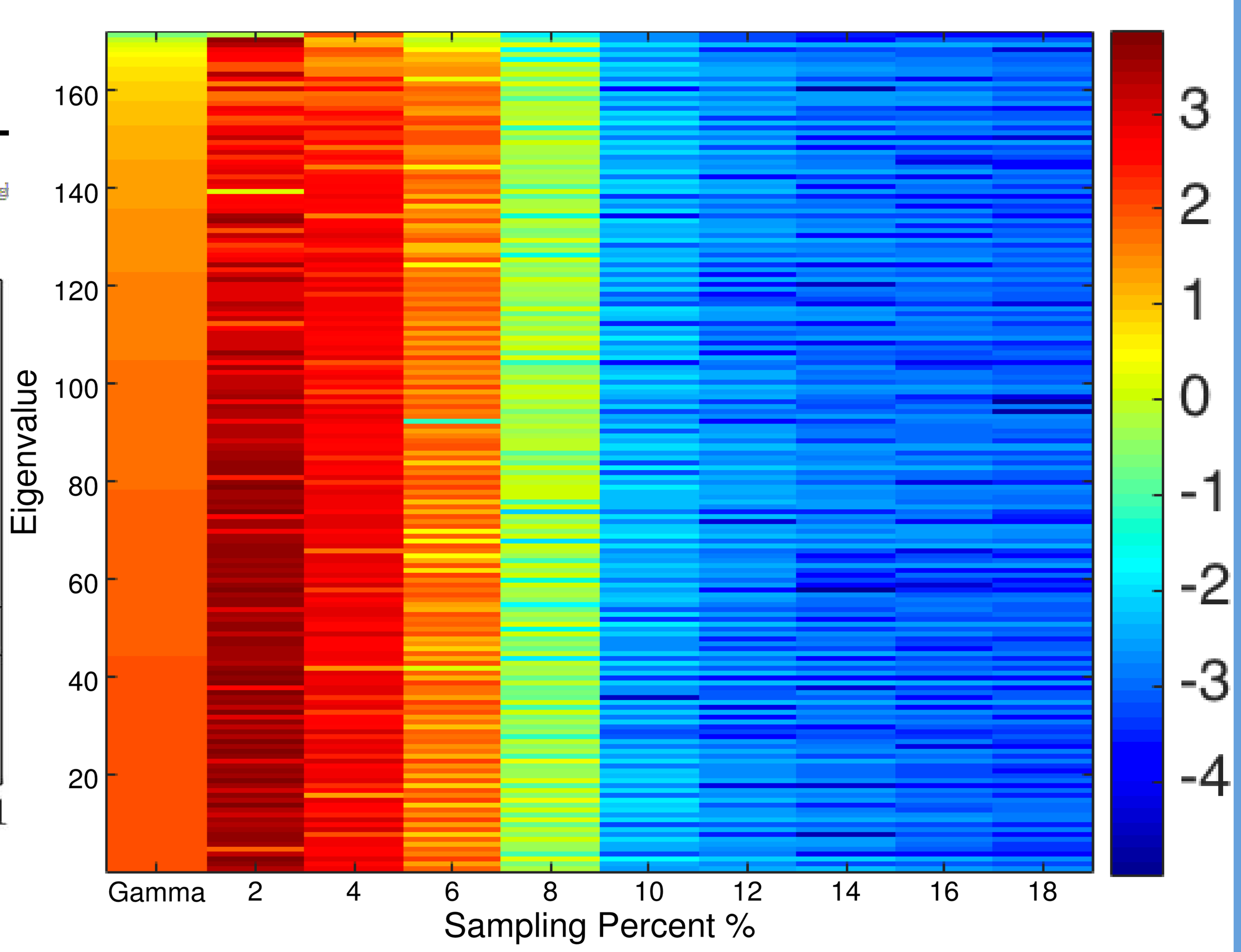
$V(x) = V_0$ for $a - L < x < a$; 0 for $0 < x < a - L$.

$V_0 = 0.459, a = 3.779, L = 2.834$ a.u.

$H(\Gamma)$ vs. $H(X)$ errors in a.u.

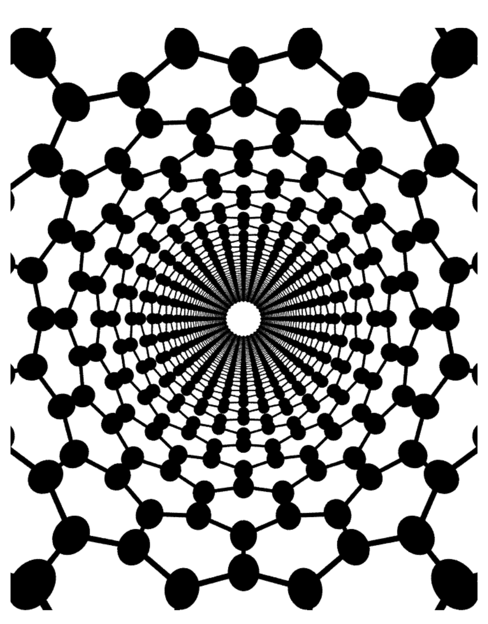




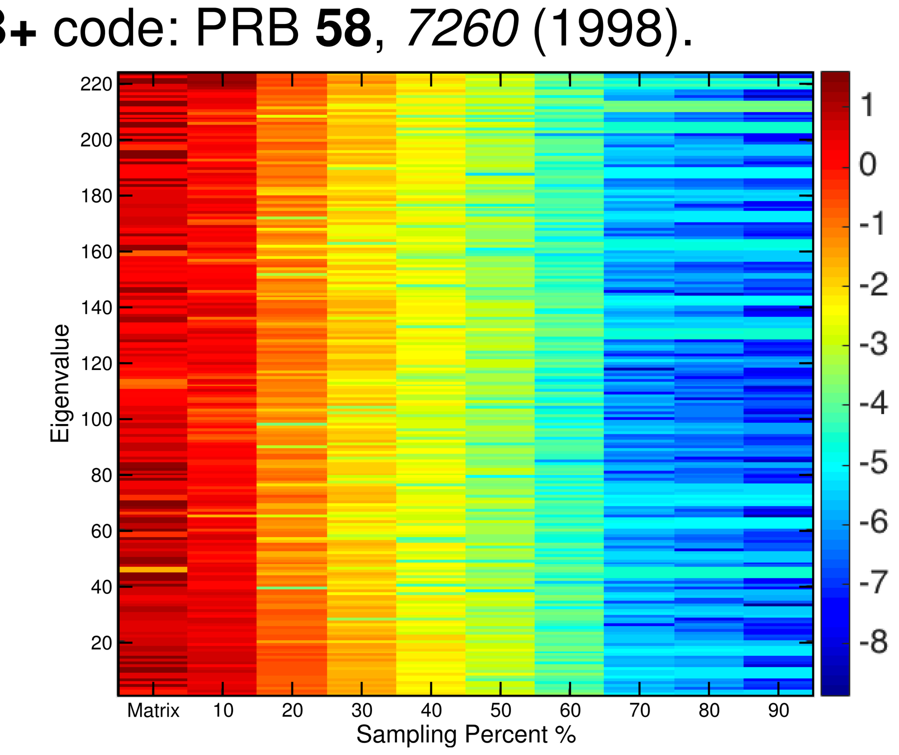


(F) (14,0) carbon nanotube: tight-binding

56 C atoms/unit cell, diameter 1.1065 nm.
DFTB+ code: PRB **58**, *7260* (1998).

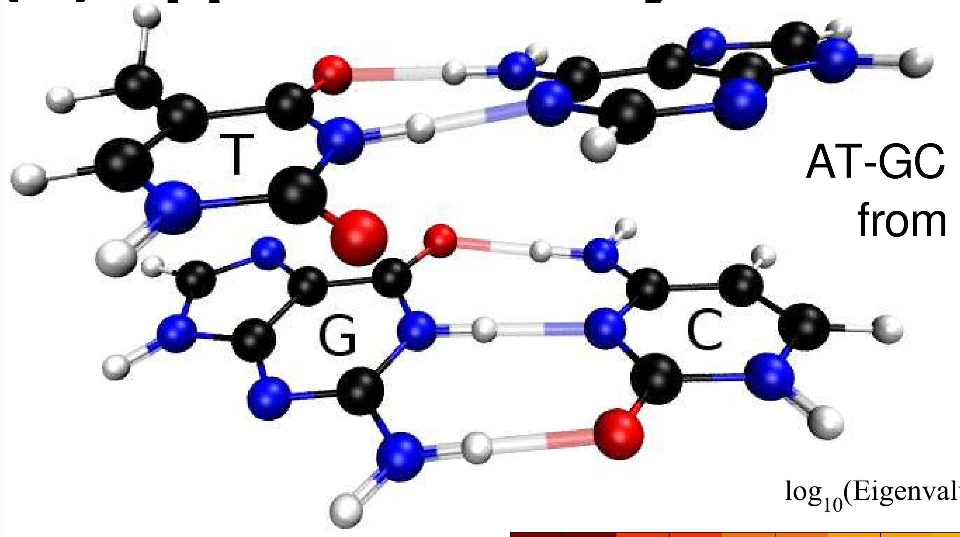


Errors in eV

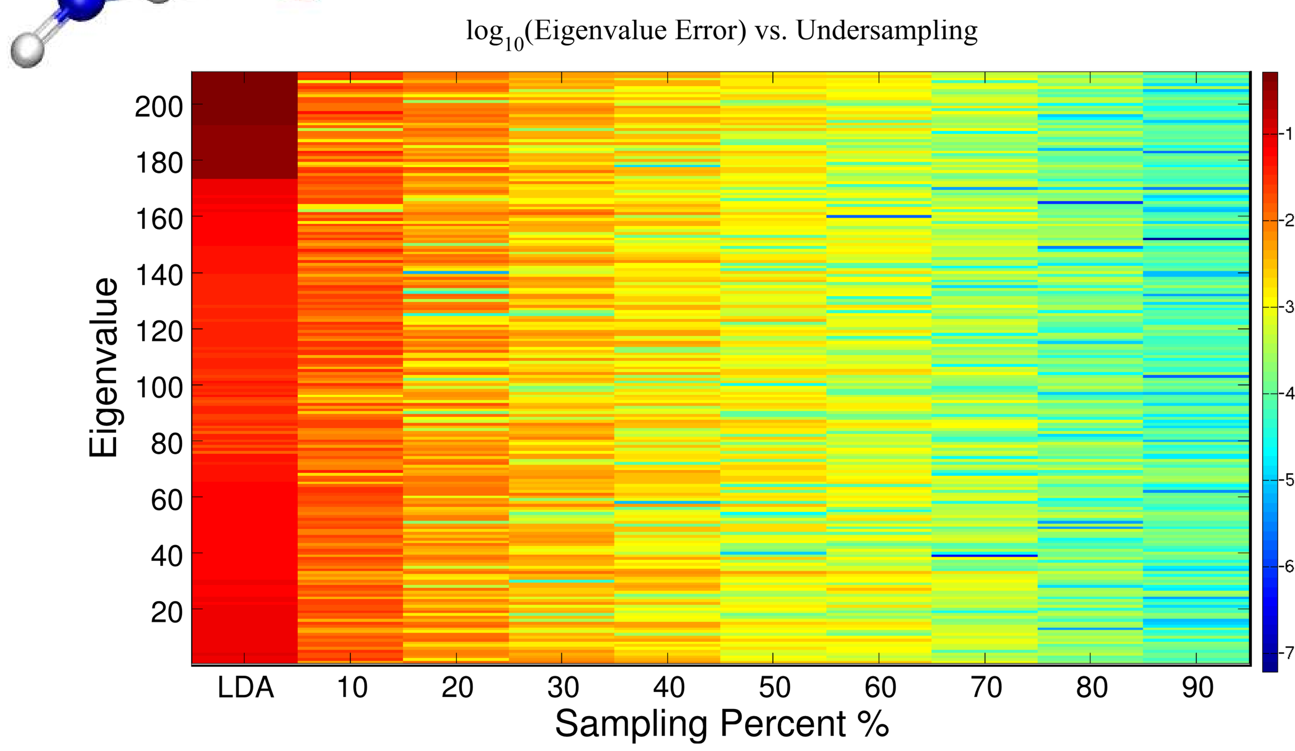


Compressed Sensing recovers sparse matrices regardless where non-zeros are.

(G) Application to hybrid PBE0/B3LYP Fockians



AT-GC Watson-Crick stacked base pairs from JPCB **114**, *1191-1203* (2010).
Errors in a.u.



We accurately recover all matrix elements with as low as 40 % of undersampling.

(H) Future Research Plan

- Investigate electron-phonon coupling matrix elements.
- Solving +Dyson Equation, Hubbard Hamiltonian?
- Application to other matrix problems in physics/chemistry.

Publications:

- X. Andrade, J. N. Sanders, & A. Aspuru-Guzik. Application of compressed sensing to the simulation of atomic systems. PNAS **109**, *35* (2012). arXiv: 1205.6485.
- J. N. Sanders, X. Andrade, & A. Aspuru-Guzik. Compressed Sensing for the Fast Computation of Matrices: Application to Molecular Vibrations. ACS Cent. Sci. **1** (1) *24-32* (2015).

Acknowledgments:

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