Problems in Computational Chemistry

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§1. Numerical mathematics

1. (10) Make iteration $x \to 1/x^2$ converging.
2. (10) Make iteration $\boldsymbol{x} \to \left(\begin{smallmatrix} 2 & 3 \\ -1 & -2 \end{smallmatrix}\right) \boldsymbol{x}$ converging.
3. (20) For a hermitian matrix H its spectral density is given by $\rho(E) = \theta(E-H)$. Find the iteration procedure for calculating ρ using only matrix addition and multiplication.
4. (20) Find "the best" orthogonal transformation connecting two sets of vectors.
5. (10) Determine "the best" Slater determinant approximating a given one-electron density matrix.
6. (20) Evaluate $\left(\begin{smallmatrix} -1 & 2 & -1 \\ -8 & 8 & -4 \\ -6 & 5 & -2 \end{smallmatrix}\right)^{1/2}$.
7. (20) Propose a complete basis set for tetrahedron potential box.
8. (10) Approximate hydrogen 1s orbital by GTO.

§2. Computational geometry

1. (20) Propose an algorithm for superposing two similar molecules (e.g. for visual comparison).
2. (20) Propose an algorithm for superposing two chemically identical molecules (e.g. for determining relative deformation).
3. (20) Propose an algorithm for determining if two molecules are chemically identical.
4. (10) Propose an efficient algorithm for determining the contact distance between two molecules.
5. (5) Reduce a lattice given by translation vectors $(4,1,2)$, $(1,1,0)$, $(5,2,1)$.
6. (30) Determine voids in As_2Se_3 crystal.
7. (5-30) Determine what Ag surface is shown on this STM image. What is wrong with that image? Analyze the linear transformations between the image and the actual Ag surface.

§3. Computational chemistry

1. (10-60) Propose a series expansion for the PES of the dihedral in biphenyl. Parametrize it using ab initio calculations. Calculate the effective mass. Solve the effective 1D Hamiltonian beyond the harmonic approximation.
2. (30) Propose a series expansion for the PES of the two most flexible dihedrals in stilbene.
3. (20) Determine bond stretching parameters for C-C σ-bond in trans-polycetylene without taking into account the π-system using ab initio calculations.
4. (30) Show that for H_2 molecule in the minimal basis there exist an "exact" semiempirical Hamiltonian.
5. (15) Create such an initial geometry that in MD only one vibrational mode will be activated.
6. (20) Benchmark density functionals for excited states.
7. (20) Benchmark semiempirical methods for geometry.
8. (10) Check if there is an energy drift in the code you use.
9. (10) Add new atom type to MM3 force field: iodide (anion).
10. (10) Add missing parameters to MM3 force field for modeling 2-thienylpyridine.
11. (20) Add missing parameters to MM3 force field for modeling N,N,N-Trimethylanilinium (cation).
12. (5) The calculations of vibrational normal modes of 2-(2-fluorophenyl)thiophene in cis conformation resulted in the following $3N$ normal mode frequencies (cm^{-1}, negative means imaginary): -28, -0.003, -0.001, 0.001, 2.8, 4.0, 5.4, 100, 167, ..., 3287. What can you say about these normal modes just looking on their frequencies?

§4. Molecules

1. (30) Find the four lowest energy Al_{13} clusters.
2. (60) Investigate the stability and aromaticity of annulenes $C_{2n}H_{2n}$.
3. (60) Create a torus from graphene. Investigate its stability and electronic properties.
4. (60) Study the solvatochromism of the Brooker's merocyanine.
5. (60) Functionalize PPV oligomer to obtain a halochromic molecule.
6. (60) Is it possible to determine the conformation of Th-PT-DTS-PT-Th molecule using UV-Vis spectra?
7. (60) Photoisomerization of azobenzene.

§5. Crystals

1. (30-99) Surface reconstruction for group-IV semiconductors: explain 7×7 reconstruction of Si(111) surface.
2. (10) Why γ-Fe is more ductile than α-Fe?
3. (30) Slice up As crystal. Investigate semiconductor to semimetal transition with the growing number of 2D layers.
4. (30-99) Semiconductor to semimetal transition for pnictides: compare black-P and α-As structures.
5. (30-99) Materials for phase change memory: investigate crystal to amorphous transition for As, GeTe, and $Ge_2Sb_2Te_5$.
6. (20) Explain α-Sn to β-Sn transition.
7. (20) Explain diamond-C to graphite-C transition.
8. (20) Explain the ferroelectric transition in $BaTiO_3$.
9. (20) Explain the ionic superconductor transition in AgI.
10. (30-99) Halogen bonds: explain the structure of bromine crystal.
11. (30-99) Explain structural trends across actinides (unit cell structure and volume, melting temperature).
12. (60-99) Can valence electrons be localized in voids of high-density crystals?
13. (60-99) Compare zincblende and wurtzite crystal structure for III+V semiconductors.

§6. Liquids and amorphous solids

1. (30) Equilibrate a water box (MM3 force field).
2. (30-99) Hydrogen bonds in water: are they essential?

§7. Complex materials

1. (30-99) Semiconductor quantum dots for optoelectronics: investigate size dependence of optical properties of Si quantum dots in SiO_2 matrix.
2. (99) Design a donor-acceptor architecture for organic solar cells.
3. (99) Investigate metallic chains on Si surface.
4. (99) Investigate chemical functionalization of graphene and graphene nanoribbons.
5. (60) Evaluate the stretching strength of carbon nanotubes.
6. (60) Evaluate mechanical properties of DNA.
7. (30) Evaluate the barrier for hydrogen to penetrate graphene.
8. (99) Fullerenes for hydrogen storage.