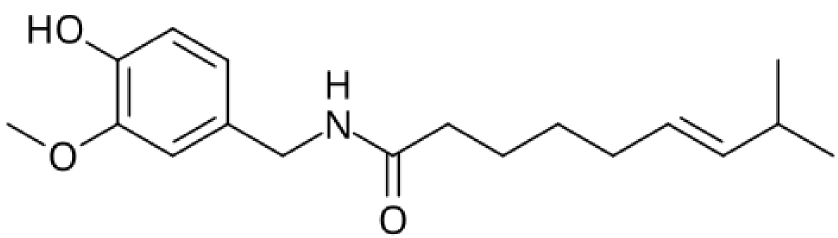
Kaiser Science Olympiad Invitational 2026

Division C

MATERIALS SCIENCE



Team Name ______________________________

Team Number __________

Honolulu
2026

Introduction

This test will largely take inspiration from the work of Yoichiro Kato at Kokuritsu Kenkyū Kaihatsu Hōjin Rikagaku Kenkyūsho (RIKEN) in Wakō, Japan. The Kato group is interested in the development and engineering of photonic and optoelectronic devices that would allow for manipulation of quantum states, as well as understanding the underlying physics in the operation of such devices, focusing on devices that utilize individual single-walled carbon nanotubes (SWCNTs) and atomically-thin layered materials.

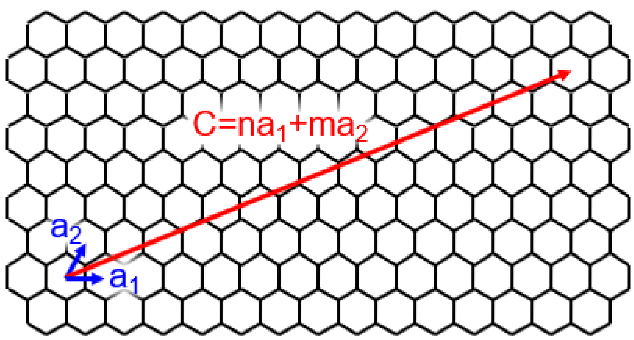
IMPORTANT: You will be provided with background information on this research. Without this information, it might be difficult to answer some questions. Therefore, you are suggested to work through this test in order (i.e. test portion before lab I, lab I before lab II, etc).

1 Molecular and electronic band structure (20 points)

1. (2 points) Fill in the blanks.

   A sheet made of carbon atoms arranged in a honeycomb lattice is known as ____________. SWCNTs have the structure of a tube made by rolling up such a sheet. SWCNTs are an example of a ___D nanomaterial.

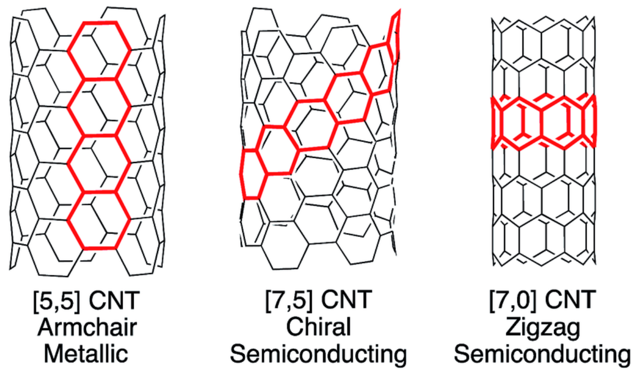
   In order to form a seamless tube, you would need to take two hexagons in a planar lattice and overlap them. A vector connecting the centers of the two hexagons is called the chiral vector, and it determines the structure of a single-walled carbon nanotube. A chiral vector can be written as $\mathbf{C} = na_1 + ma_2$ where a_1 and a_2 are basis vectors of the graphene lattice. The pair of integers (n, m) is called the chiral index (or chirality).

   The most interesting aspect of SWCNTs is that their electronic structure can become either semiconducting or metallic depending on chirality.

2. (3 points) Fill in the blanks.

   In the sheet, each carbon atom has ___ hybridization; three orbitals form σ bonds with neighboring carbon atoms in a planar hexagonal lattice, and one remaining p_z orbital (perpendicular to the plane) forms the π and π^* bonds responsible for __________. The curvature introduced by rolling up the sheet alters orbital orientations. The p_z orbitals are no longer perfectly perpendicular to the surface, σ and π orbitals are no longer orthogonal, and there is a mixing between σ and π states. As a result, carbon atoms in carbon nanotubes (CNTs) exhibit partial ___ character, often described as $sp^2 + \delta$ hybridization.



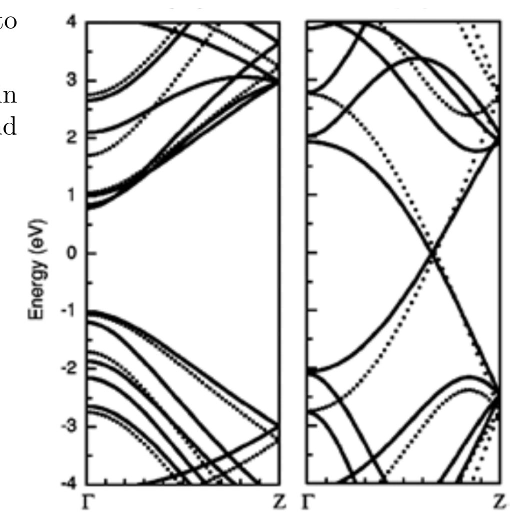
Above are some SWCNTs with nice properties. In general, SWCNTs with chirality (n, n) are called armchair, and those with $(n, 0)$ are called zigzag.

3. (1 point) What does the bandgap of a material represent?

4. (1 point) What would be the bandgap of an ideal armchair SWCNT? ___ eV

5. (1 point) Circle the SWCNT band diagram that is more likely to be a zigzag.

6. (3 points) What is the name given to the $E = 0$ energy level in band structure diagrams such as the ones shown on the right, and what does it represent?



7. (3 points) Fill in the blanks.

In the context of band structures, Γ and Z represent high-__________ points in the first ________ zone in reciprocal space. In the same way the ________ lattice is divided up into Wigner-Seitz cells in real space, the reciprocal lattice is broken up into these zones.

The sheets have a hexagonal lattice with primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$. The Dirac points are located at $\mathbf{K} = \frac{1}{3}(\mathbf{b}_1 - \mathbf{b}_2)$, $\mathbf{K}' = -\mathbf{K}$. At these points, the conduction and valence bands touch, so the sheets are gapless. Rolling the sheets into cylinders imposes a periodic boundary condition around the circumference:

$$\mathbf{k} \cdot \mathbf{C} = 2\pi\ell$$

for some integer ℓ, where $\mathbf{C}$ is the chiral vector. This condition restricts allowed wavevectors to parallel lines in k-space.

8. (1 point) What are these lines called?

A nanotube is metallic if and only if one allowed **k**-line passes through a Dirac point, requiring $\mathbf{K} \cdot \mathbf{C} = 2\pi\ell$. While all armchair nanotubes are metallic, not all zigzag nanotubes are semiconducting.

9. (3 points) Using the information you have about electronic band structure in CNTs, show why the SWCNT with chirality $(3, 0)$ is metallic. (You might find the reciprocal relation $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$ useful)

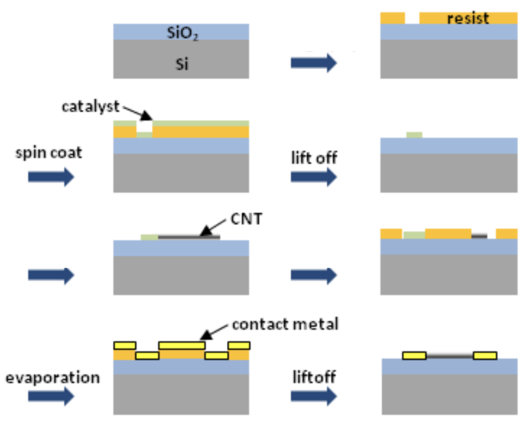
10. (2 points) Semiconducting CNTs have direct bandgaps. What does this mean in terms of the crystal momentum of electrons and holes?

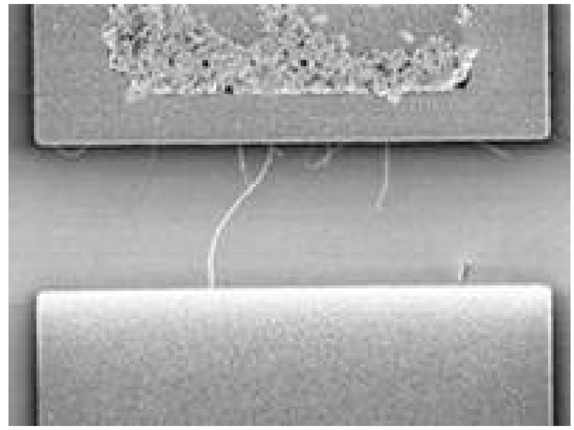
2 Production and characterization (8 points)

11. (1 point) Which of the following techniques is most commonly used to produce CNTs?
    A. Sol-gel process
    B. Chemical vapor deposition
    C. Spin coating
    D. Electroplating

12. (1 point) A known limitation of the technique above in CNT synthesis is:
    A. Formation of defects
    B. High equipment cost
    C. Limited control over nanotube length
    D. Very low yield

13. (1 point) Which of the following characterization techniques can provide a quantitative estimate of CNTs' metal contents or impurities?
    A. SEM
    B. TEM
    C. STM
    D. EDX





While it is difficult to put electrical contacts on a molecule or a dot, CNTs are long enough to be used to make electronic devices. One such device produced by the Kato group is the field effect transistor (FET). The device fabrication process is diagrammed above (left), and an image of a CNT FET is provided (right).

14. (2 points) What is the name of the technique used by the Kato group to produce CNT FETs? Is it a top-down or a bottom-up method?

15. (1 point) Which characterization technique was most likely used to produce the image of the CNT FET provided?

    A. SEM
    B. TEM
    C. AFM
    D. Raman spectroscopy

16. (1 point) While CNT FETs are not used much in the real world, metal-oxide-semiconductor FETs (MOSFETs) are by far the most common transistor in digital circuits, as billions may be included in a memory chip or microprocessor. Why does the metal–oxide used in MOSFETs simplify production and characterization compared with CNT FETs?

    A. It forms a native, chemically stable oxide directly from silicon.
    B. It enables higher intrinsic carrier mobility in the channel than CNTs.
    C. It eliminates the need for surface-sensitive characterization techniques.
    D. It relies on reversible charge-transfer doping.

17. (1 point) Which characterization technique is useful for MOSFETs but generally not applicable to CNT FETs?

    A. XRD
    B. Raman spectroscopy
    C. AFM
    D. XPS

3 Concrete (6 points)

If you competed in materials science last year, you probably made concrete from Portland cement. An interesting real-world application of CNTs is in concrete.

18. (1 point) Which fundamental type of chemical bonding gives CNTs their exceptionally high tensile strength?
    A. Ionic bonding
    B. Metallic bonding
    C. Hybridized covalent carbon-carbon bonding
    D. Hydrogen bonding

19. (1 point) Which hydration phase in cement is most likely to benefit from nanoscale interfacial interactions with CNTs due to its poorly crystalline structure?
    A. Calcium hydroxide
    B. Ettringite
    C. Calcium silicate hydrate
    D. Monosulfate

20. (1 point) CNTs can accelerate cement hydration primarily because their surfaces:
    A. Act as preferential adsorption sites for ionic species
    B. Chemically decompose clinker phases
    C. Increase diffusion rates of silicate anions
    D. Convert calcium hydroxide into C−S−H

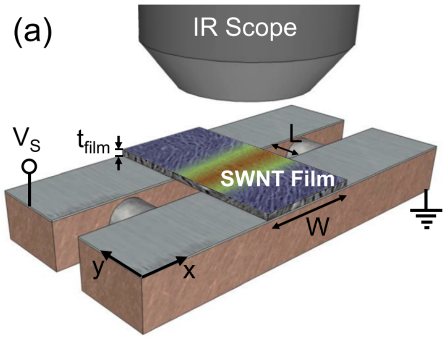
21. (1 point) Poor CNT dispersion in cement paste is detrimental because agglomerates:
    A. React preferentially with calcium hydroxide
    B. Increase electrical resistivity of the matrix
    C. Accelerate carbonation reactions
    D. Reduce effective surface area for interfacial interactions

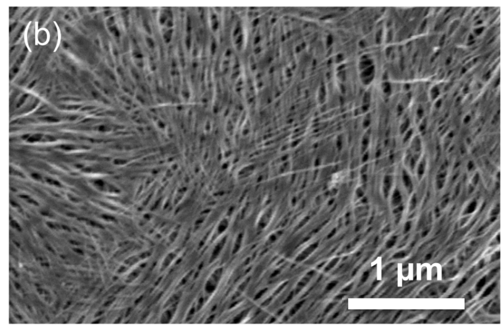
22. (1 point) The strong tendency of CNTs to cluster in aqueous cement systems arises mainly from:
    A. High surface energy and van der Waals attractions
    B. Coulombic attraction between charged tube ends
    C. Covalent crosslinking under alkaline conditions
    D. Hydrogen bonding with pore water molecules

23. (1 point) Another widely used nanomaterial that enhances concrete properties is nanosilica (nano-SiO_2), which refines pores, reduces permeability, accelerates hydration, and improves resistance to chemical attack and abrasion. Which of the following types of nanomaterials is nanosilica?
    A. Ceramic nanomaterial
    B. Metal-oxide nanomaterial
    C. Covalent nanomaterial
    D. Carbon-based nanomaterial

4 Thermal properties (10 points)

While the Kato group is more interested in photonics and optoelectronics, some groups, such as Eric Pop's lab at Stanford University, work with SWCNTs in the context of thermoelectrics. In this section, we will consider a study of the Pop lab done on SWCNT films, that is, 2D networks of SWCNTs. On the right is (a) a schematic of the thermometry platform and experimental setup, with SWCNT films suspended across two Pd-coated Cu blocks electrically isolated by ceramic washers, and (b) an image of the SWCNT film after vacuum filtration, with SWCNTs bundled and randomly in-plane oriented.





24. (1 point) In a network of SWCNTs, which heat carriers are expected to dominate thermal transport at room temperature?
    - A. Free electrons, due to metallic nanotubes
    - B. Phonons, due to lattice vibrations in the nanotubes
    - C. Photons, due to strong infrared absorption
    - D. Magnons, due to spin transport along nanotubes

25. (1 point) Why is the geometry of this setup (films suspended between two large metal contacts) particularly useful for extracting in-plane thermal conductivity?
    - A. It maximizes radiative heat loss
    - B. It enforces approximately one-dimensional heat flow
    - C. It eliminates electrical contact resistance
    - D. It increases the emissivity of the film

26. (1 point) Why is IR thermal imaging well suited for measuring temperature profiles in suspended SWCNT films?
    - A. IR imaging directly measures phonon population
    - B. It eliminates the need for thermal modeling
    - C. It allows direct measurement of thermal conductivity
    - D. It provides spatially resolved, non-contact temperature measurements

27. (1 point) In the study, the metallic SWCNT films contain shorter nanotubes on average than the semiconducting films. From a heat transport perspective, shorter nanotubes would tend to:
    - A. Increase thermal conductivity by reducing phonon scattering
    - B. Increase electronic heat conduction
    - C. Reduce thermal conductivity by increasing junction density
    - D. Have no effect because phonons travel ballistically

28. (1 point) The Pop lab compared films made from mostly metallic, mostly semiconducting, and unsorted SWCNTs. From a materials perspective, which factor would you expect to most strongly affect thermal conductivity in such films?

    A. Electronic band structure (metallic vs semiconducting)

    B. Optical absorption coefficient

    C. Network morphology (density, junction density, alignment)

    D. Work function differences between nanotubes

29. (1 point) Why is it necessary to account for electrical contact resistance when extracting thermal conductivity from Joule-heating experiments?

    A. It changes the emissivity of the film

    B. It alters the phonon dispersion in the nanotubes

    C. It affects how much power is actually dissipated in the suspended film

    D. It determines the nanotube chirality distribution

30. (1 point) The study finds that films with higher mass density generally show higher in-plane thermal conductivity. Which explanation best accounts for this trend?

    A. Higher density increases electronic carrier concentration

    B. Higher density improves thermal coupling between nanotubes

    C. Higher density reduces the number of nanotube junctions

    D. Higher density suppresses radiative heat losses

31. (1 point) Based on general heat-transfer principles, increasing nanotube alignment in the plane of the film would most likely:

    A. Increase in-plane thermal conductivity

    B. Increase cross-plane thermal conductivity only

    C. Have no effect on thermal conductivity

    D. Decrease thermal conductivity

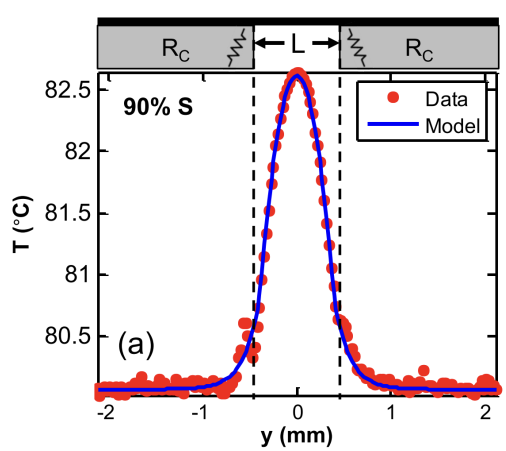
32. (1 point) The figure to the right shows temperature profiles that peak near the center of the suspended SWCNT film during Joule heating. What does this shape most directly indicate?

    A. Non-uniform electrical current injection

    B. Strong heat sinking at the metal contacts

    C. Radiative heat loss dominating conduction

    D. A phase transition in the nanotube network



Film Type	**σ (S/m)**	**R_{sh} ($\Omega/\square$)**	**$2R_C W$ ($\Omega\cdot$mm)**	**L_T (mm)**
90%-S	$\sim 8.34 \times 10^4$	~ 26	~ 35.0	~ 0.65
90%-M	$\sim 1.17 \times 10^5$	~ 20	~ 6.35	~ 0.16
Unsorted	$\sim 1.22 \times 10^5$	~ 16	~ 0.34	~ 0.10

Thermal conductivities ($W \cdot m^{-1} \cdot K^{-1}$)

Sample	**Metallic**	**Semiconducting**	**Unsorted**
1	106.2	174.1	116.7
2	112.5	182.9	138.8
3	121.1	185.6	130.6
4	136.7	220.2	288.3

33. (1 point) The upper table above gives electrical and physical properties for the 90% semiconducting, 90% metallic, and purified unsorted SWCNT films in the Pop study. The lower table gives extracted thermal conductivities for various SWCNT film types in the same study. Based on this data, does SWCNT chirality significantly control the thermal conductivity of the films? Explain your reasoning by comparing the estimated electronic contribution to thermal conductivity from the Wiedemann–Franz law to the total thermal conductivity. (It is not sufficient to look only at the measured thermal conductivities of the metallic, semiconducting, and unsorted films because those values reflect multiple coupled effects, not chirality alone; Wiedemann-Franz isolates the only chirality-dependent heat transport channel)

5 Lab I: excitons (15 points)

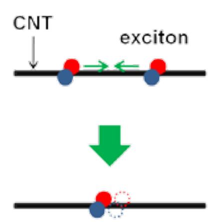
You will analyze data produced by the Kato group. In this first dry lab, you will explore the exciton physics of suspended CNTs.

IMPORTANT: You will need to use your data sheet for the lab sections. We refer to figures in the problem statements; those figures are provided and labeled in the data sheet.

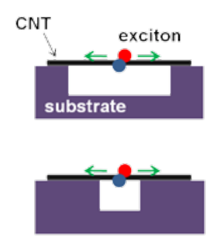
Coulomb interaction is strong in SWCNTs because of the one-dimensional structure, causing the formation of tightly bound excitons. (An exciton is a bound state of an electron and a hole attracted to each other by Coulomb force; it is an electrically neutral quasiparticle. For an exciton to be tightly bound means that there is a small separation and large binding energy between the electron and hole.) A process called exciton-exciton annihilation determines the optical emission efficiency. This process happens when two excitons collide, and it results in one of the excitons to nonradiatively decay into ground state. The rate at which these collisions occur is set by the spatial range that the excitons traverse through diffusion. The diffusion length of excitons (that is, the average distance an exciton travels before recombining) is found by measuring photoluminescence (PL) from nanotubes suspended over trenches of various widths.

34. (3 points) What is photoluminescence? How does it occur in terms of electrons and holes, and at what energy?

The process of exciton-exciton annihilation and exciton diffusion is diagrammed to the right. The substrate induces a very rapid nonradiative decay of excitons, serving as a sink for excitons. With mobile excitons (longer diffusion lengths), the dominant nonradiative recombination occurs at the contacts between nanotubes and the substrate, as manifested in the length dependence of PL intensities. This is known as end quenching, and this significantly reduces the emission efficiency when the diffusion length is longer than the nanotube length.



Exciton-exciton annihilation



Exciton diffusion

35. (2 points) Referring to figure 1(b) in your data sheet, what physical processes do the two resonances correspond to in nanotube spectroscopy?

36. (2 points) In figure 1(c-d), satellite spots appear at slightly lower energy than main spots. Propose a plausible physical explanation.

37. (2 points) Using figure 2, what does a longer diffusion length imply about exciton motion? How does diffusion length influence how strongly PL depends on nanotube length?

38. (3 points) Using figure 3 (for (9,7) tubes), explain the following:

    i Why does PL intensity increase rapidly with length for short nanotubes?

    ii Why does PL intensity level off (saturate) for long nanotubes at low excitation power?

    iii Why does increasing excitation power change the shape of the curve?

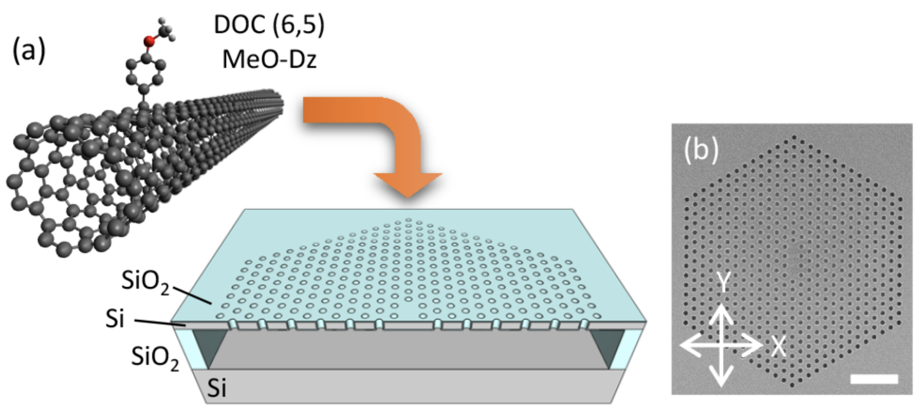
39. (3 points) Using figure 4, what does it mean when PL intensity increases linearly with excitation power? Why does PL increase more slowly than linear at high power? What physical process is responsible for this change?

6 Lab II: single-photon emission (13 points)

In this second dry lab, you will explain the physics behind a real application of SWCNTs.

Single-photon emitters are important in quantum information technologies. SWCNTs are regarded as a promising material for such an application because they are a nanoscale light-emitting material having stable excitonic states.

SWCNTs can be intentionally modified with sp^3-bonded dopant sites, creating localized electronic states below intrinsic nanotube exciton energy acting as exciton traps.



(a) Schematic images of a 4-methoxybenzenediazonium-doped (6,5) SWCNT and a photonic crystal microcavity. (b) A scanning electron micrograph of a photonic microcavity.

A photonic crystal cavity is a nanostructured dielectric environment that restricts which optical modes exist, enhances emission at specific wavelengths and polarizations, and alters how efficiently emitters couple to light without changing the emitter's chemistry. In Kato's work, the cavity is created by patterning a periodic array of nanometer-scale air holes into a thin silicon layer, forming a two-dimensional photonic crystal. A small, intentional break in this periodic structure—created by removing or shifting several holes—acts as a structural defect that traps light in a localized region, in direct analogy to how atomic defects trap electrons in solids.

From the previous activity, you learned that mobile excitons are quenched by diffusion to tube ends or by exciton-exciton annihilation. In contrast, localized defect excitons do not diffuse over microns, but they are still sensitive to interfaces, substrates, and local environment.

40. (2 points) Normally, defects are associated with loss. Give two reasons why introducing dopant defects in SWCNTs can increase useful photoluminescence instead of reducing it.

41. (1 point) Why might defect emission be more useful than intrinsic emission for device applications?

42. (2 points) What structural change occurs in the nanotube lattice when aryl dopants are introduced? How does this local structural change affect exciton motion along the nanotube? (An aryl is any functional group derived from an aromatic ring; an example of an aryl dopant is 4-methoxybenzenediazonium, depicted in the schematic earlier in this section)

43. (2 points) One of the big advantages of the Kato group's SWCNT single-photon emitters is their ability to operate at room temperature. The dopant-related emission appears at a lower energy than the intrinsic nanotube emission. Explain why introducing a localized structural defect would shift emission to a lower energy and make emission more stable at room temperature.

44. (2 points) Compare emission from the same nanotube on and off the cavity (figure 5e-f). What structural feature of the cavity determines which wavelengths are enhanced? Why does the same emitter show very different spectra depending on position?

45. (2 points) The PL lifetime shortens when the nanotube emission is coupled to the cavity (figure 6). Explain how changing the optical environment, without changing the nanotube itself, can alter the emission lifetime and increase light emission efficiency.

46. (1 point) Despite many nanotubes being present, the system shows strong single-photon behavior (figure 7). Explain how structural selectivity (defect localization & cavity modes) can cause one or very few emitters to dominate and suppress multi-photon emission.

47. (1 point) Tiebreaker #1, organic chemistry bonus: What is the common name of the molecule on the front of the test?

End of exam

You have reached the end of the test. This test was written by **Raphael Esquivel** ('Iolani '25, Harvey Mudd '29). Please don't hesitate to ask questions or provide comments/suggestions by emailing me: esquivelralphie@gmail.com

I am not affiliated with RIKEN, the Kato group, or the Pop lab. You can learn more about the Kato group and their work at https://katogroup.riken.jp/, and you can learn more about the Pop lab at https://poplab.stanford.edu/index.html.

The reference paper for section 4 on thermal properties is:

Lian, Feifei & Llinas, Juan & Li, Zuanyi & Estrada, David & Pop, Eric. (2016). Thermal Conductivity of Chirality-Sorted Carbon Nanotube Networks. Applied Physics Letters. 108. 103101. 10.1063/1.4942968.

All figures in section 4 were retrieved from the paper above.

The reference paper for lab I is:

Ishii, A. & Yoshida, M. & Kato, Yuichiro. (2014). Exciton diffusion, end quenching, and exciton-exciton annihilation in individual air-suspended carbon nanotubes. Physical Review B. 91. 10.1103/PhysRevB.91.125427.

All figures and data in the provided data sheet corresponding to lab I were retrieved from the paper above.

The reference paper for lab II is:

Ishii, A. & He, Xiaowei & Hartmann, N. & Machiya, Hidenori & Htoon, H. & Doorn, S. & Kato, Yuichiro. (2018). Enhanced single photon emission from carbon nanotube dopant states coupled to silicon microcavities. 10.48550/arXiv.1803.08628.

All figures in section 6 and all figures and data in the provided data sheet corresponding to lab II were retrieved from the paper above.

The electronic band diagrams were generated by Valentin Popov and were retrieved from

https://www.phys.uni-sofia.bg/~vpopov/elbscomp.htm. The reference paper is:

Popov, Valentin & Henrard, Luc. (2004). Comparative study of the optical properties of single-walled carbon nanotubes within orthogonal and nonorthogonal tight-binding models. Physical Review B. 70. 115407. 10.1103/PhysRevB.70.115407.

The armchair, chiral, and zig zag SWCNT drawings were retrieved from the following paper:

Sisto, Thomas & Zakharov, Lev & White, Brittany & Jasti, Ramesh. (2016). Towards Pi-Extended Cycloparaphenylenes as Seeds for CNT Growth: Investigating Strain Relieving Ring-Openings and Rearrangements. Chem. Sci.. 7. 10.1039/C5SC04218F.

All other figures were retrieved from the Kato group website.