Quantum collapse associated with electron tunneling in substantia nigra pars compacta (SNc) tissue

Chris Rourk (crourk@jw.com)
Hitchhiker's Advanced Guide to Quantum Collapse Models, October 31, 2022

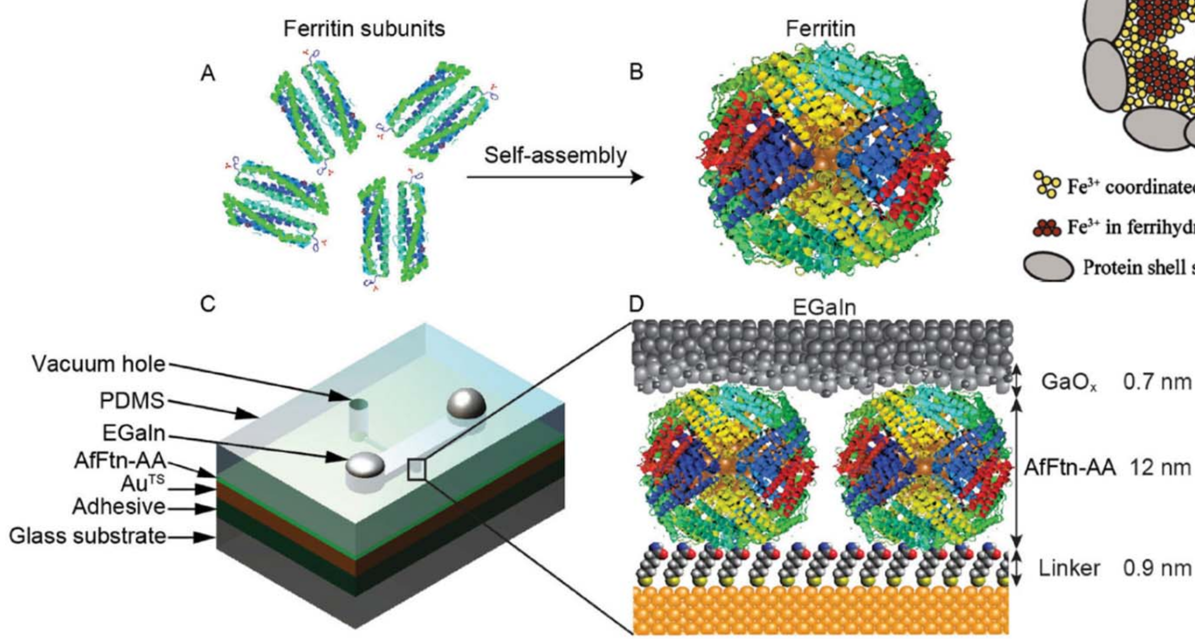
from https://en.wikipedia.org/wiki/Substantia_nigra#/media/File:Substantia_nigra.gif, CC BY-SA 4.0

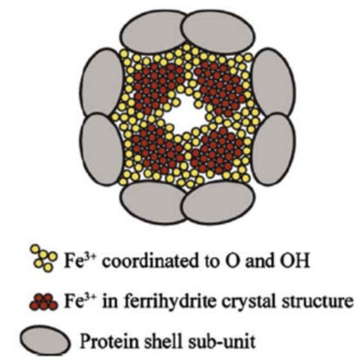
Outline of Presentation

- **Electron tunneling in ferritin**
- Ferritin in SNc tissue
- Modelling electron transport in the SNc and wave function collapse

Ferritin and long-range electron tunneling

- 24 sub-unit spherical shell (light, heavy chain, mitochondrial).
- Stores up to ~4500 Fe atoms as Fe3+.
- Electron tunneling behavior first observed 1995, room temp ~2005.
- Prof. Christian Nijhuis - coherent tunneling as a function of Fe loading.

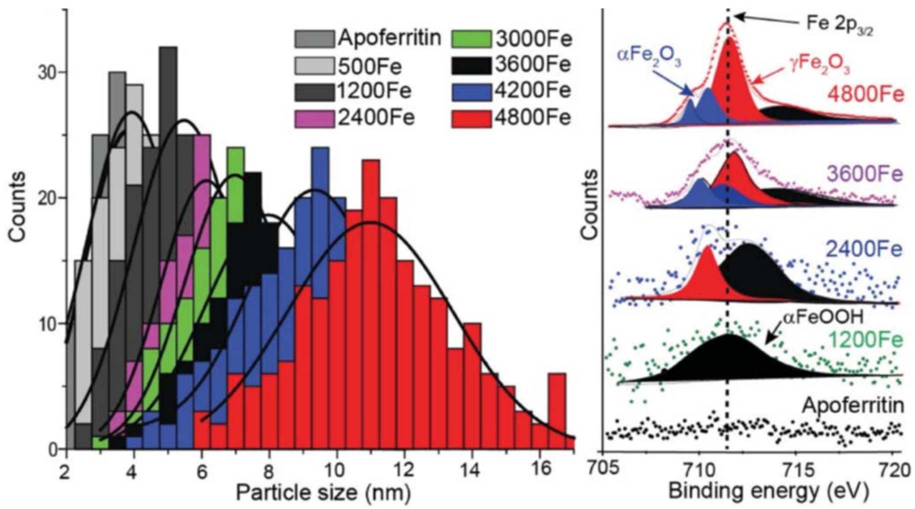


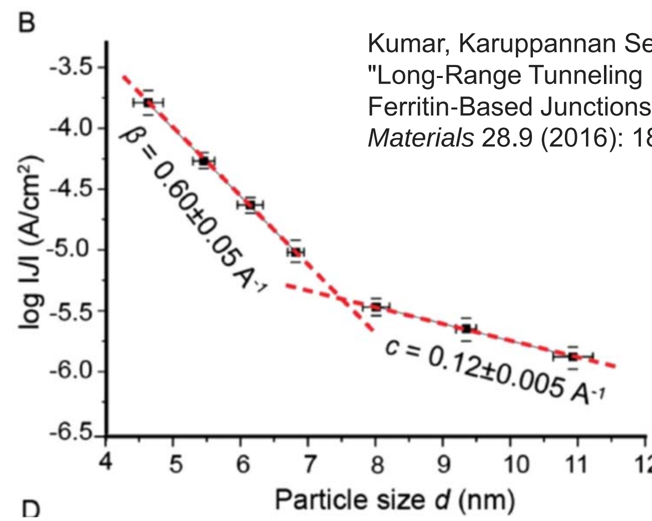


Kumar, Karuppannan Senthil, et al. "Long-Range Tunneling Processes across Ferritin-Based Junctions." *Advanced Materials* 28.9 (2016): 1824-1830.

Pan, Ying-Hsi, et al. "3D morphology of the human hepatic ferritin mineral core: New evidence for a subunit structure revealed by single particle analysis of HAADF-STEM images." *Journal of structural biology* 166.1 (2009): 22-31.

Ferritin and long-range electron tunneling

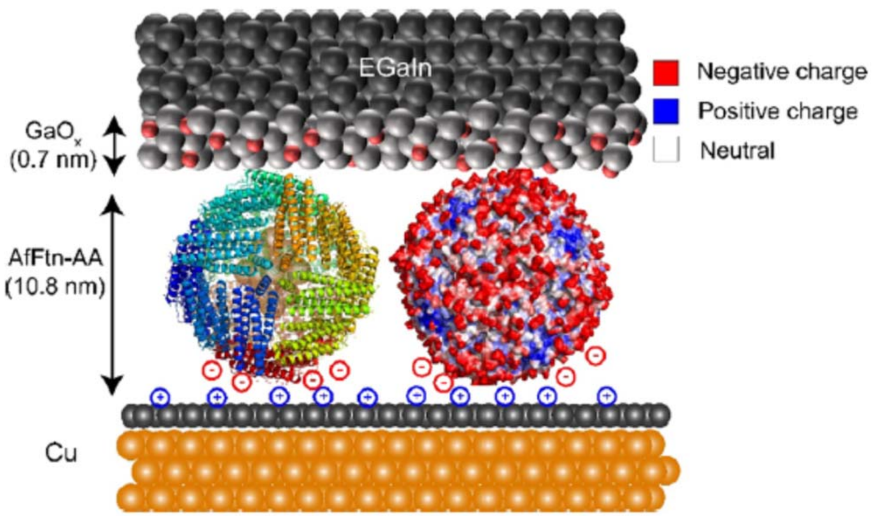


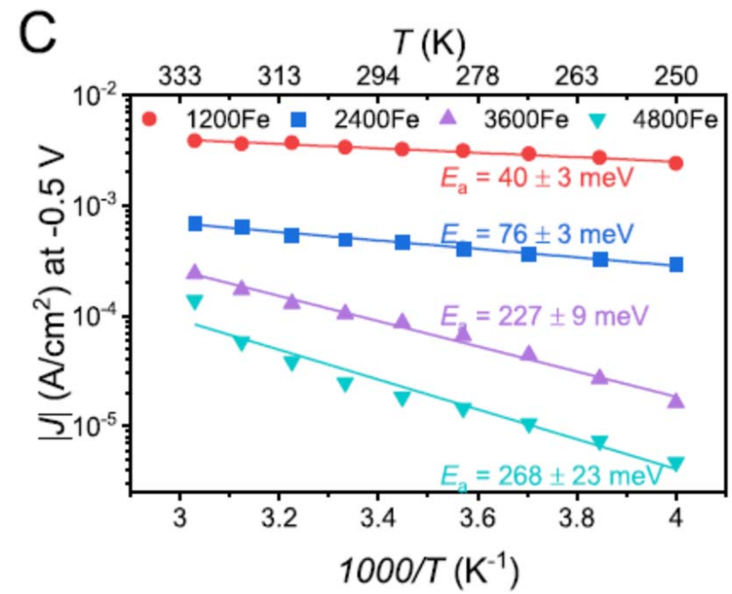


Kumar, Karuppannan Senthil, et al. "Long-Range Tunneling Processes across Ferritin-Based Junctions." *Advanced Materials* 28.9 (2016): 1824-1830.

- Size, composition of ferritin core changes with iron loading
- Tunneling parameters are a function of size
- Coherent (temperature independent) tunneling

Coherent and incoherent electron tunneling in ferritin

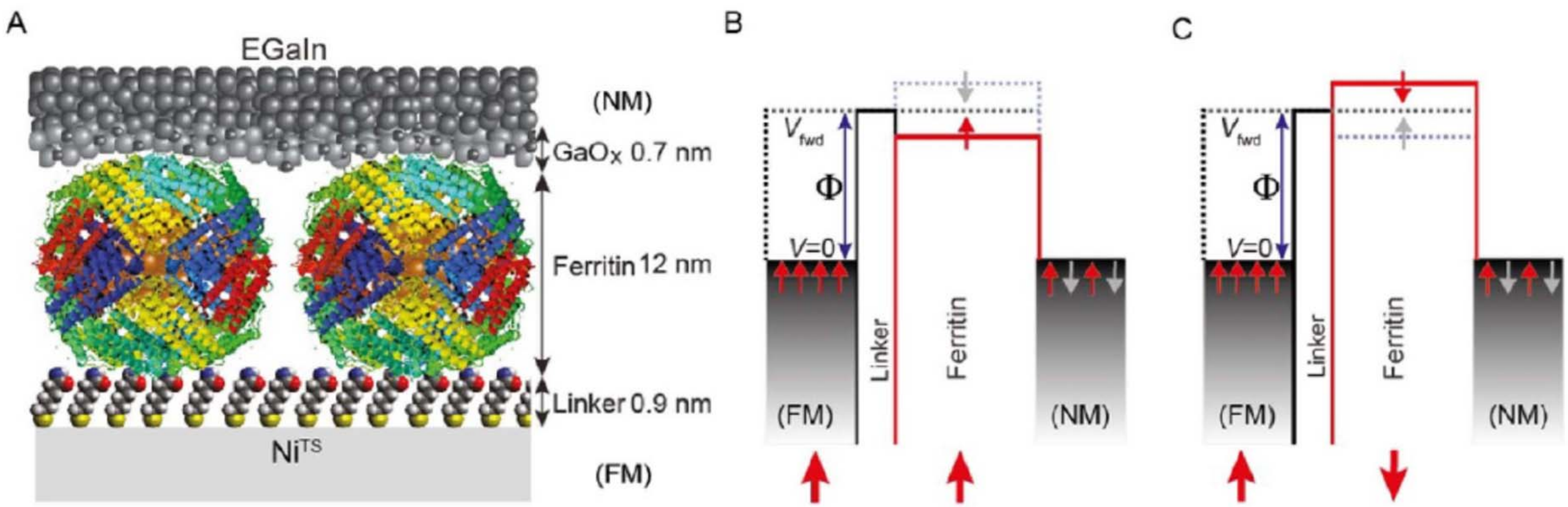




In an incoherent process, the charge carrier transiently occupies localized states. Temperature facilitates the propagation from one state to the next, yielding a generic Arrhenius dependence of current density . . . on temperature. In contrast, **coherent tunneling processes (regardless of resonance) are independent of the temperature**.

Gupta, Nipun Kumar, et al. "Temperature-Dependent Coherent Tunneling across Graphene–Ferritin Biomolecular Junctions." *ACS applied materials & interfaces* (2022).

Ferritin and magnon-assisted electron tunneling



The mechanism of charge transport across iron oxide loaded ferritin junction studied here is independent of the temperature, which suggests that a long-range tunneling mechanism of charge transport predominates. To explain the observed TMR involving large coercive fields present in the junctions, but absent in apo ferritin, **we propose that 'long-range tunneling' is assisted by magnon excitations of ferritins.**

Karuppannan, Senthil Kumar, et al. "Room-temperature tunnel magnetoresistance across biomolecular tunnel junctions based on ferritin." Journal of Physics: Materials 4.3 (2021): 035003.

Electron tunneling in ferritin as a function of Fermi level of contact material

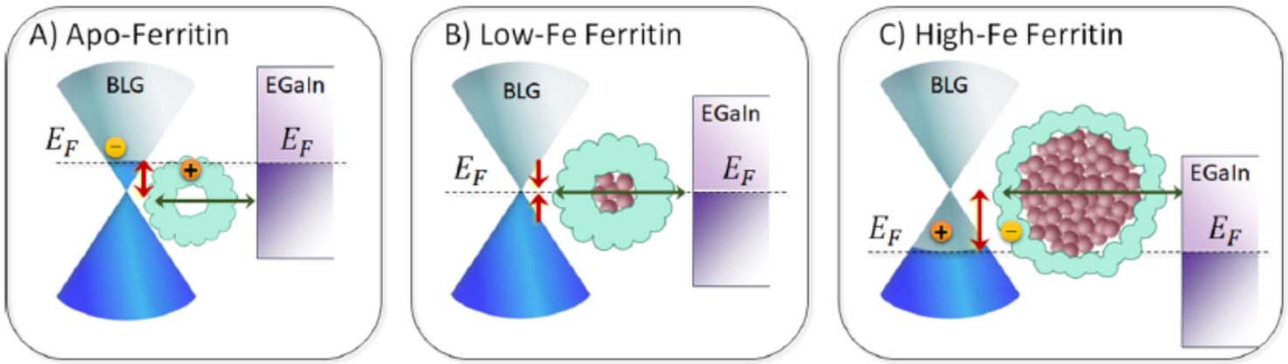
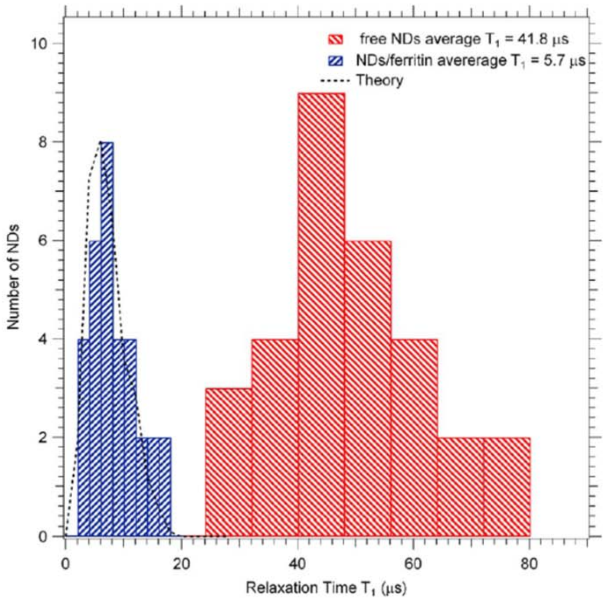
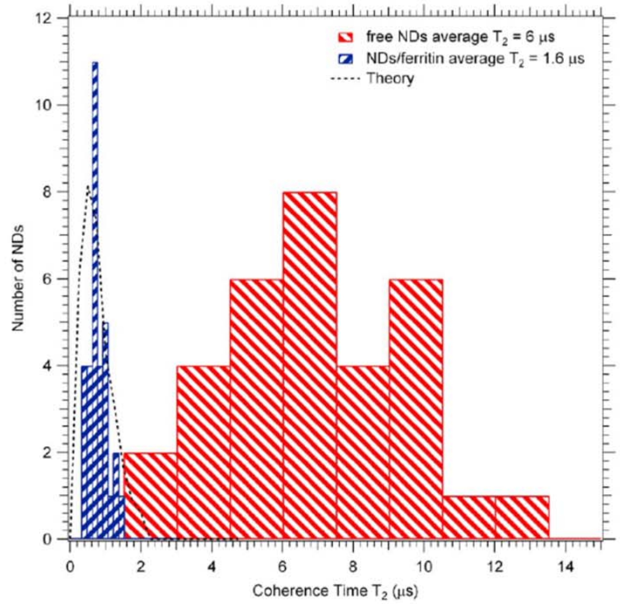


Figure 5. Schematic illustration of energy alignment between BLG (blue-gray dual cones) and (A) apo-AfFtn-AA, (B) AfFtn-AA with small iron oxide, and (C) large iron oxide core. The top-EGaIn contact (purple) is shown without an external bias. Vertical direction represents electron's energy, and the horizontal direction indicates generally the distance perpendicular to the junction, except for the BLG dual cone representing its energy dispersion with respect to momentum. The horizontal green arrow indicates coherent tunneling, and the vertical red arrow indicates the energy barrier (ε_0), which varies due to interfacial charging (indicated with the "+" and "−" signs) that shifts the graphene's Fermi level (E_F). The cone-shaped energy dispersion of graphene implies that small shifts in E_F translate to exponential changes in the density of available carriers.

Gupta, Nipun Kumar, et al. "Temperature-Dependent Coherent Tunneling across Graphene–Ferritin Biomolecular Junctions." *ACS applied materials & interfaces* (2022).

Ferritin – electron spin characteristics



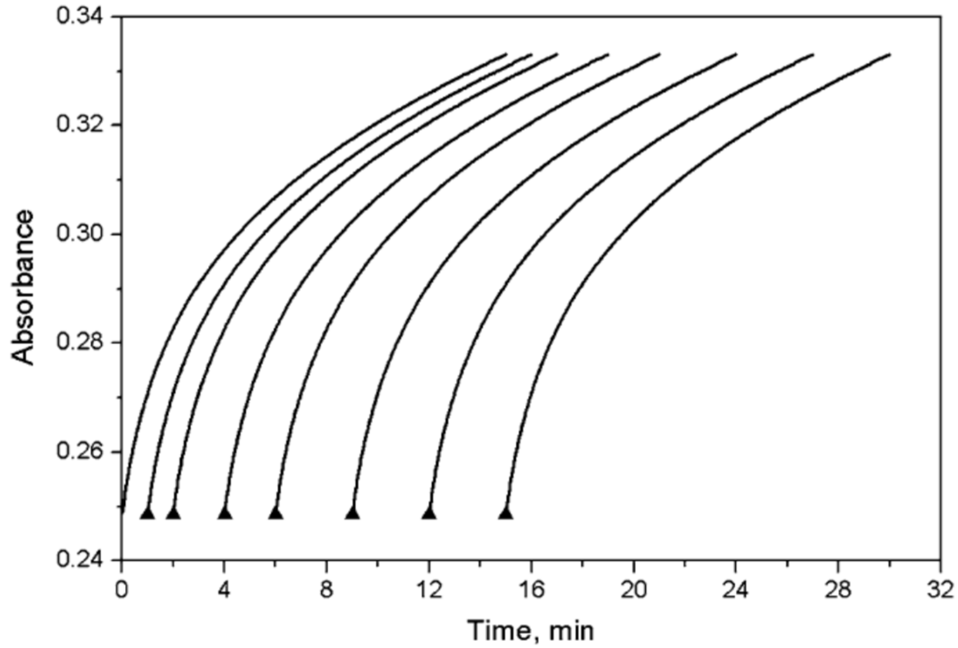


Ermakova, A., et al. "Detection of a few metallo-protein molecules using color centers in nanodiamonds." Nano letters 13.7 (2013): 3305-3309.

- Effect of ferritin cores on nanodiamond nitrogen vacancy (N.V.) spins.
- Relaxation time T1 and spin coherence time T2 reduced by ferritin attached to nanodiamonds at room temperature.

Ferritin – electrical characteristics

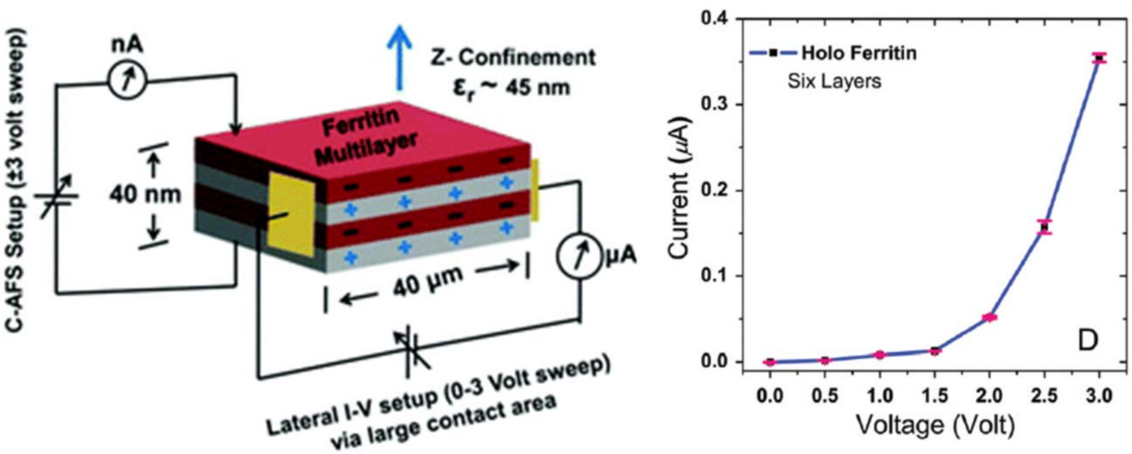
- Electrons loaded onto ferritin cores with e-beams (linear accelerator), laser pulses (308 nm)
- “Without a chelator, ferritin is an electron-storage molecule for a long period, on the order of at least several hours.”
- How many electrons?



Wolszczak, Marian, and Joanna Gajda. "Iron release from ferritin induced by light and ionizing radiation." *Research on chemical intermediates* 36.5 (2010): 549-563.

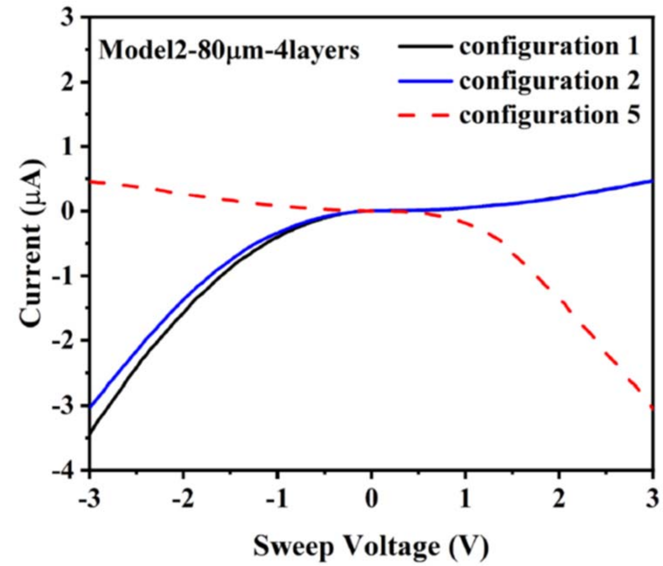
Electron tunneling through disordered ferritin arrays at room temperature

0.3 microamperes across 40 microns at 3 volts



Bera S., Kolay J., Pallabi Pramanik P., Bhattacharyyab A., Mukhopadhyay R. (2019), Long-range solid-state electron transport through ferritin multilayers. J. Mater. Chem. C, 7, 9038-9048.

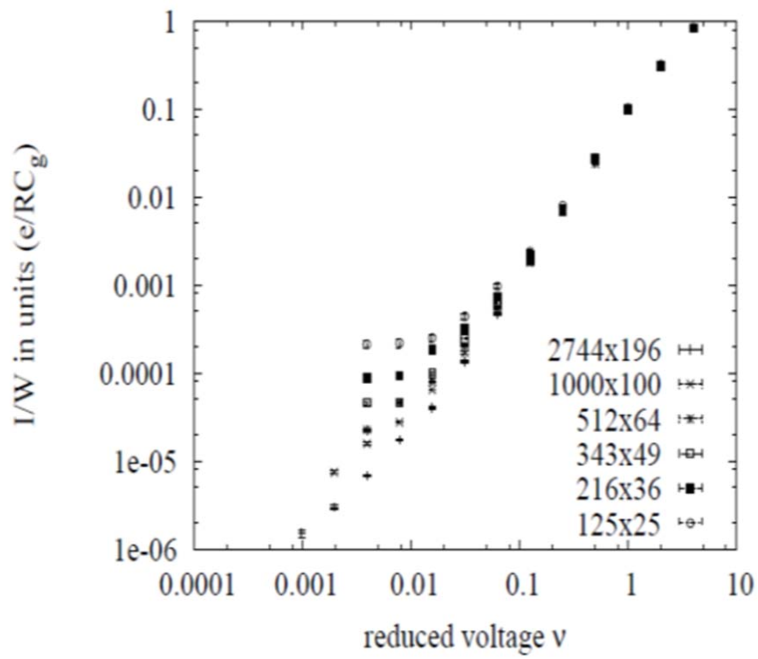
3 microamperes across 80 microns at 10 volts



Rourk, Christopher, et al. "Indication of Strongly Correlated Electron Transport and Mott Insulator in Disordered Multilayer Ferritin Structures (DMFS)." Materials 14.16 (2021): 4527.

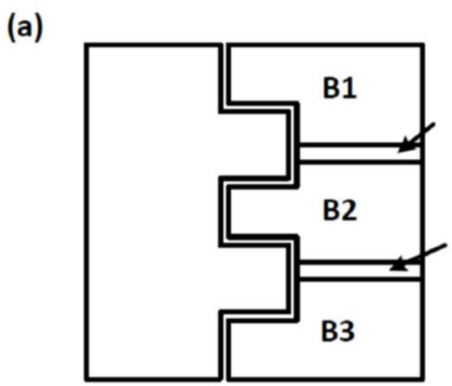
Electron tunneling between electrodes through disordered quantum dot arrays

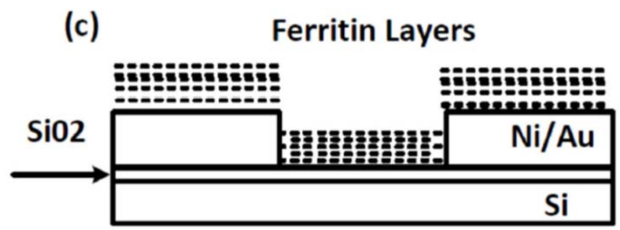
- Treats quantum dots as islands separated by capacitances, with wave functions localized to a single dot, other simplifying assumptions.
- Ignores temperature effects for tunneling probability (T=0)



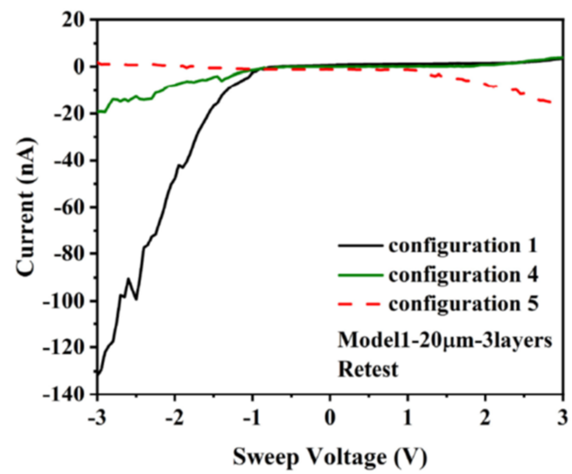
Jha A, Middleton A (2012), Effects of Disorder on Electron Transport in Arrays of Quantum Dots, arXiv:cond-mat/0511094

Switching/routing in disordered ferritin arrays





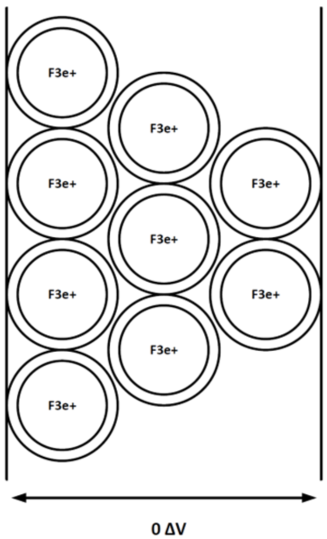
Rourk, Christopher, et al. "Indication of Strongly Correlated Electron Transport and Mott Insulator in Disordered Multilayer Ferritin Structures (DMFS)." Materials 14.16 (2021): 4527.



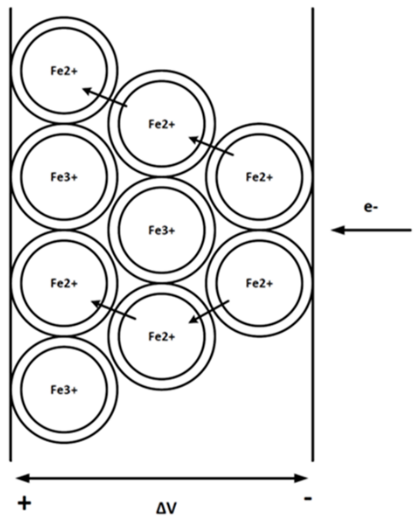
- Different switching configurations tested
- Disordered multilayer ferritin structures were not consistent but multiple dies exhibited switching/routing

~$10,000

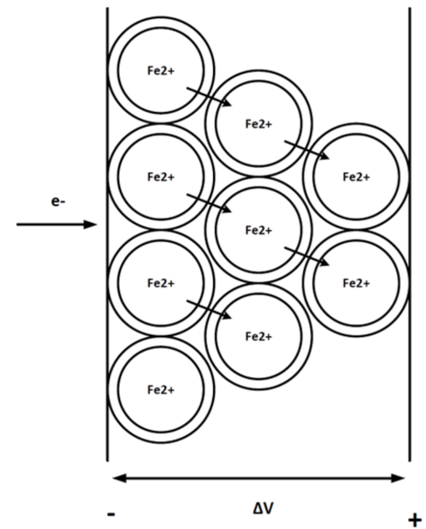
Coulomb blockade behavior of ferritin



0 ΔV - Iron in +3 oxidation state



Iron in +3 and +2 oxidation states



Iron in +2 oxidation state

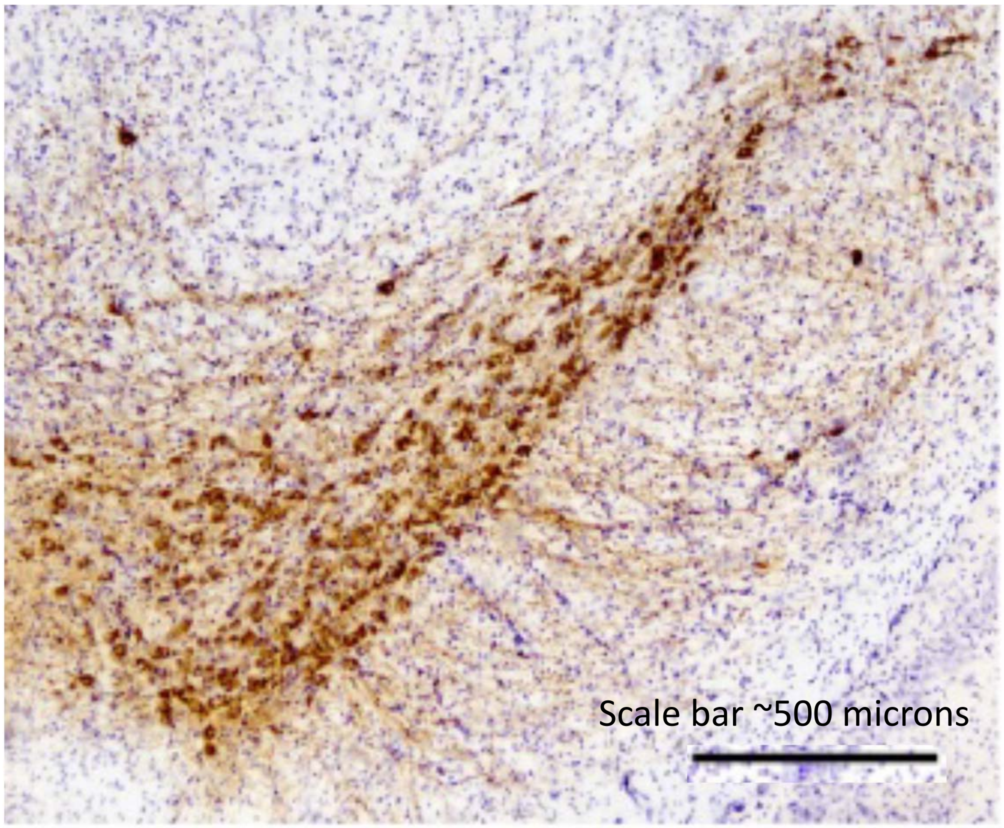
- **Coulomb blockade results in strong electron-electron interactions that can integrate information.**
- **“Excellent agreement between the experimental data and the Coulomb blockade theory is demonstrated.”**

Labra-Muñoz, Jacqueline A., van der Zandt et al. "Ferritin-Based Single-Electron Devices." *Biomolecules* 12.5 (2022): 705.

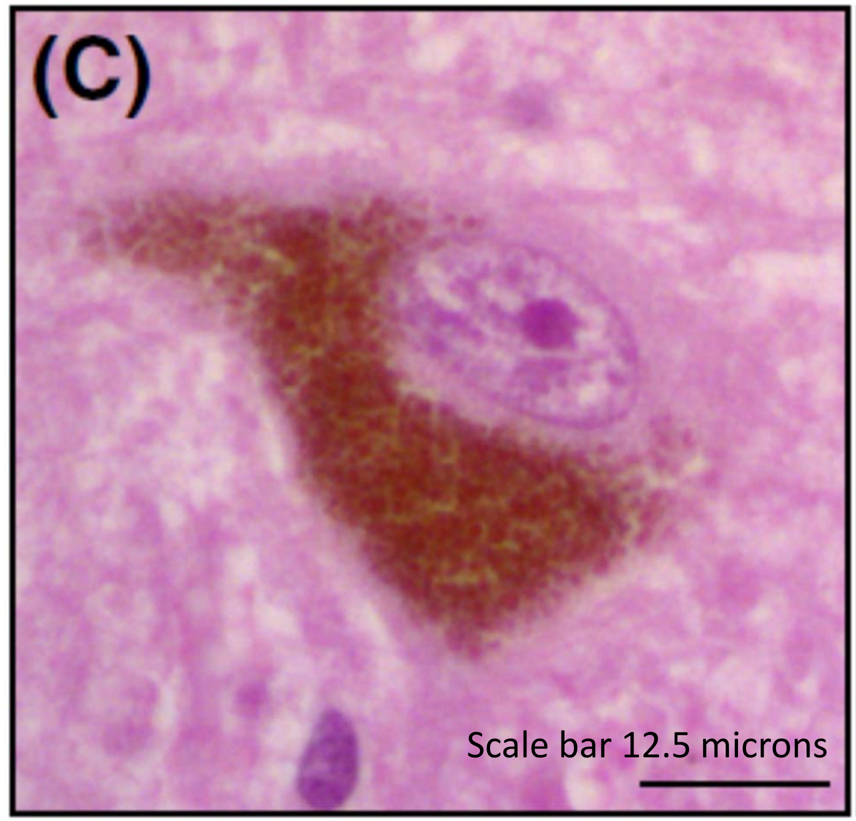
Outline of Presentation

- Electron tunneling in ferritin
- **Ferritin in SNc tissue**
- Modelling electron transport in the SNc and wave function collapse

SNc large dopamine neurons and neuromelanin

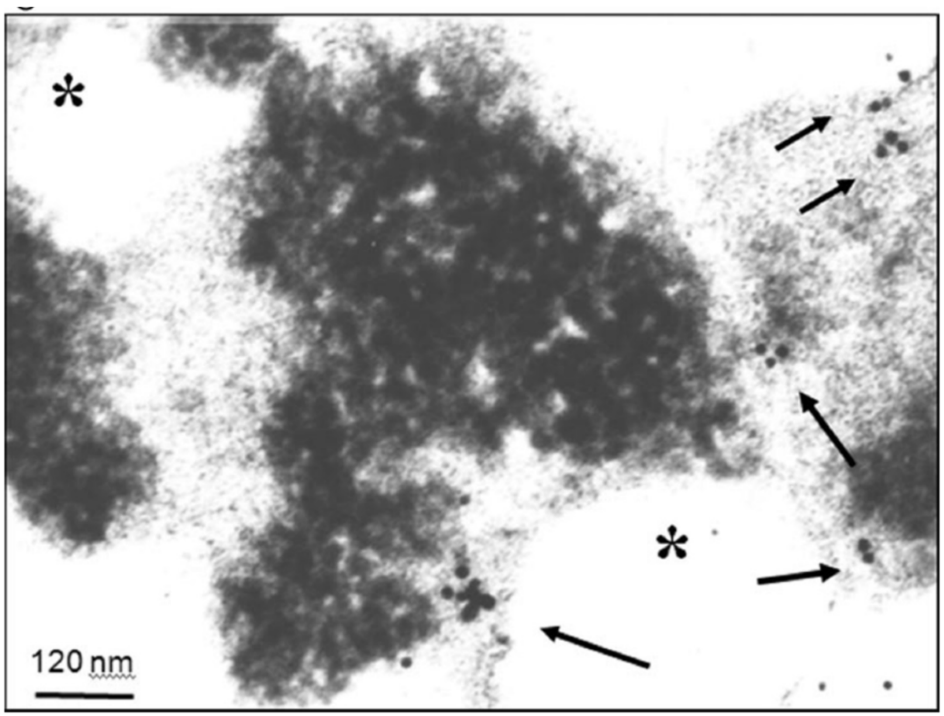


Grathwohl, Stefan, et al. "Experimental colitis drives enteric alpha-synuclein accumulation and Parkinson-like brain pathology." *bioRxiv* (2019): 505164.



Vila, Miquel. "Neuromelanin, aging, and neuronal vulnerability in Parkinson's disease." *Movement Disorders* 34.10 (2019): 1440-1451.

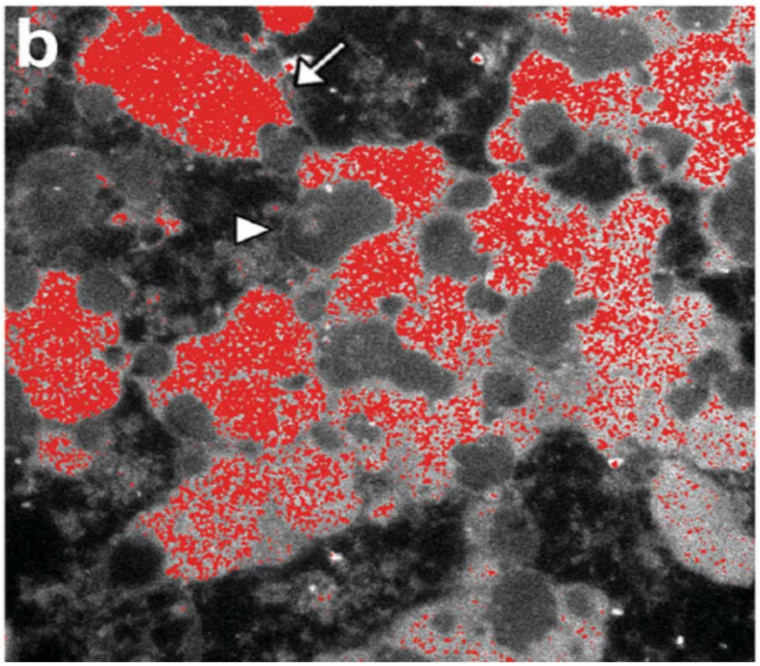
Ferritin outside of NMOs in large dopamine neurons



Tribl, Florian, et al. "Identification of L-ferritin in neuromelanin granules of the human substantia nigra: a targeted proteomics approach." *Molecular & Cellular Proteomics* 8.8 (2009): 1832-1838.

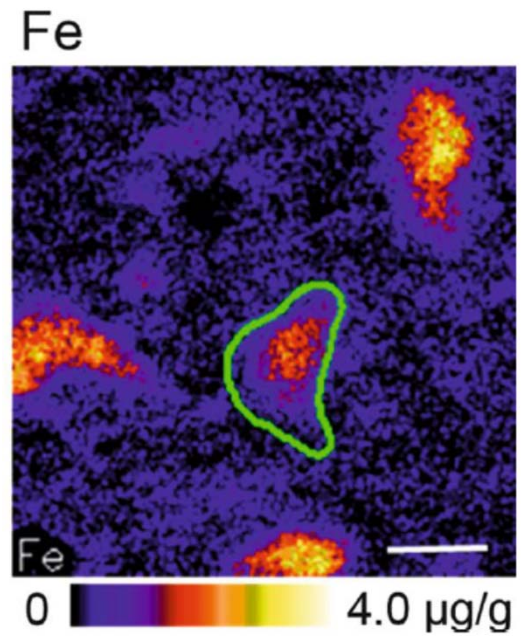
Disordered ferritin arrays in SNc tissue

Layers of iron outside neuromelanin organelles (electron spectroscopy)



Sulzer, D. et al. Neuromelanin Detection by Magnetic Resonance Imaging (MRI) and Its Promise as a Biomarker for Parkinson's Disease. Parkinson's Disease 2018, 4, 11

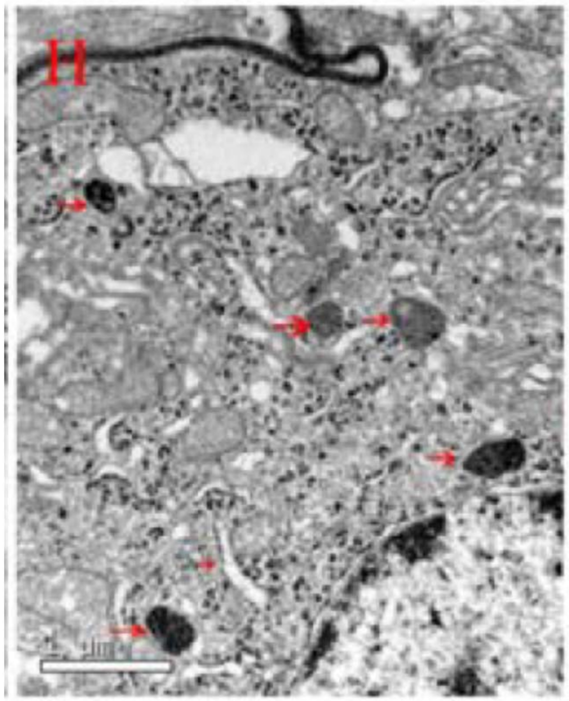
Iron is present in, and in continuous regions between, SNc dopamine neurons (particle-induced X-ray emission)



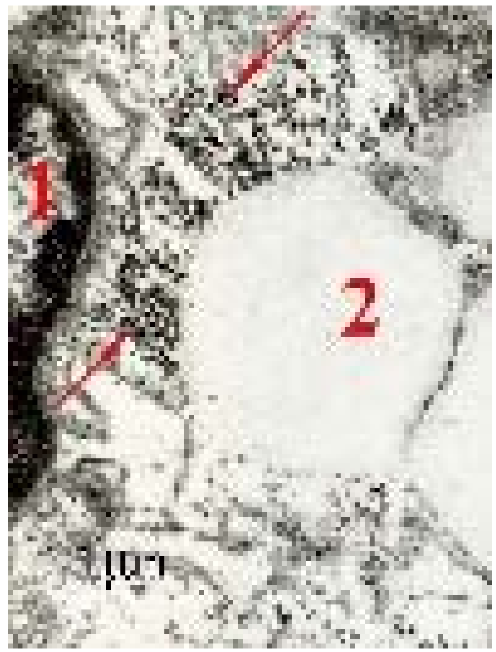
Friedrich, I., et al. "Cell specific quantitative iron mapping on brain slices by immuno-µPIXE in healthy elderly and Parkinson's disease." *Acta Neuropathologica Communications* 9.1 (2021): 1-17.

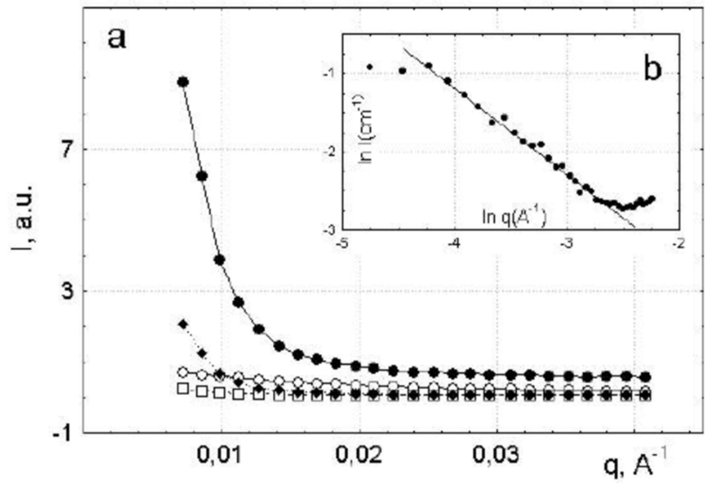
Ferritin arrays in SNc glial cells

Layers of ferritin inside SNc glial cells



Xiong, Nian, et al. "Stereotaxical infusion of rotenone: a reliable rodent model for Parkinson's disease." *PloS one* 4.11 (2009): e7878



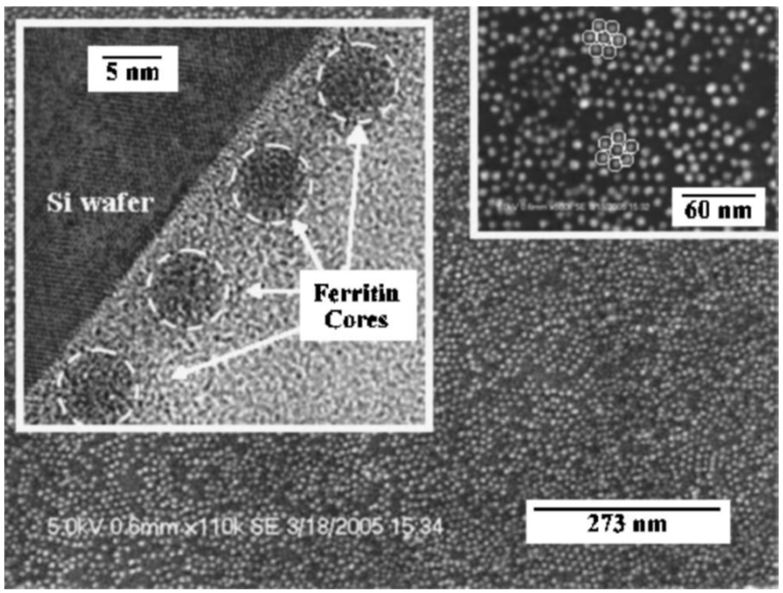


Mykhaylyk, Olga, et al. "On the magnetic ordering of the iron storage proteins in tissues." *Journal of magnetism and magnetic materials* 272 (2004): 2422-2423.

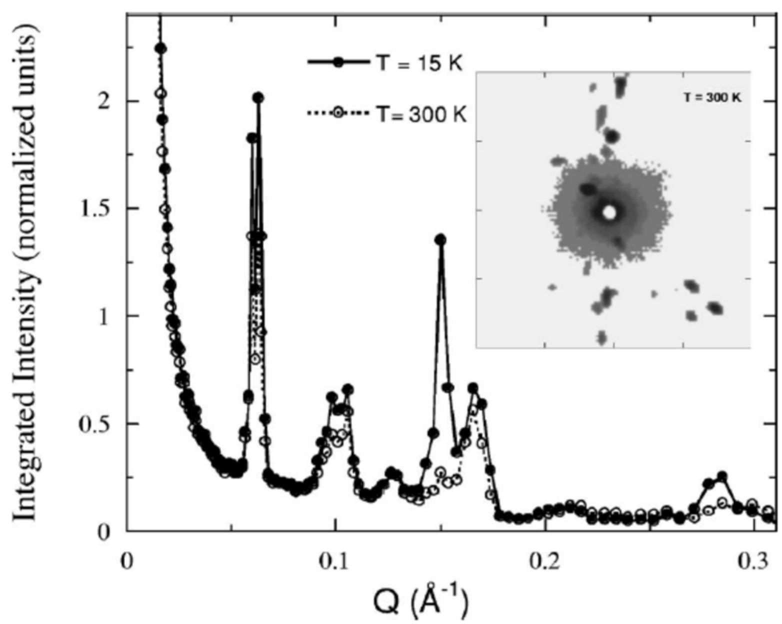
"Small angle scattering (both X-ray [SAXS] and neutron [SANS]) have provided quantitative structural insight into a range of QDs systems . . ."

Toolan, Daniel TW, et al. "Controlling the structures of organic semiconductor–quantum dot nanocomposites through ligand shell chemistry." *Soft Matter* 16.34 (2020): 7970-7981.

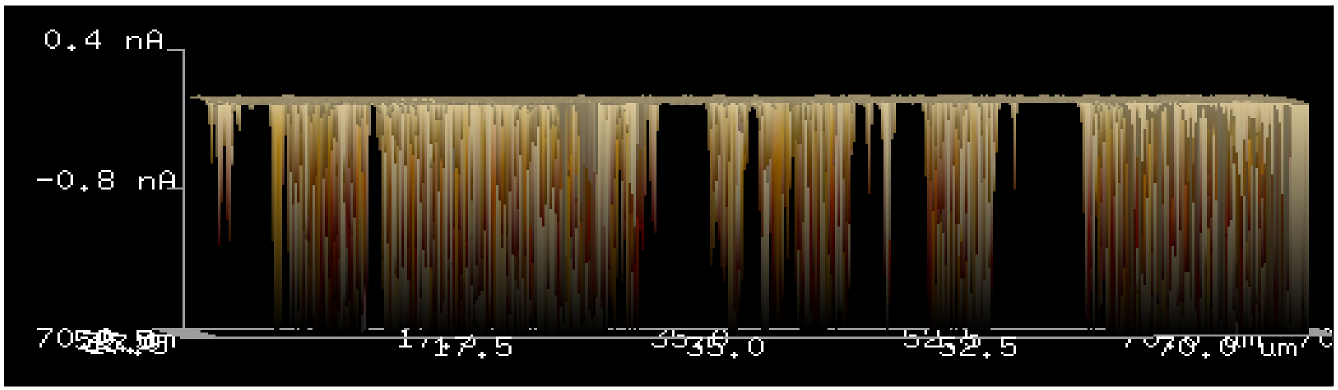
Ordered ferritin cores have increased magnetic ordering

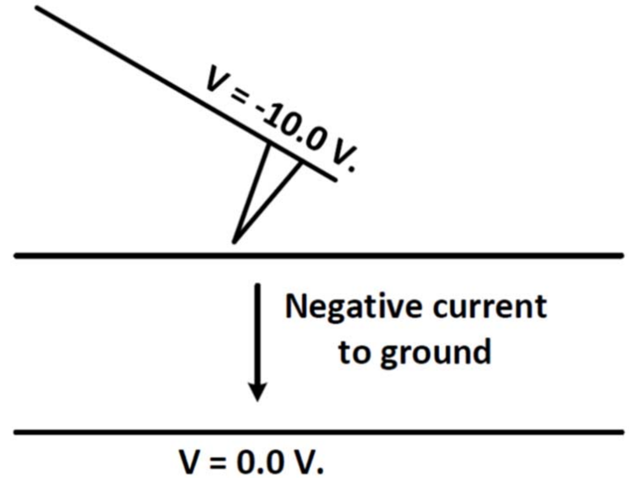


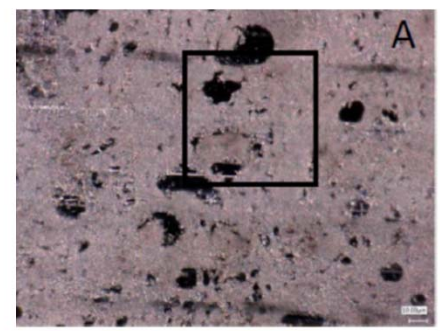
Yuan, Zhen, Nakotte, Heinz et al. "Magnetic properties of self-assembled ferritin-core arrays." *Journal of applied physics* 99.8 (2006): 08Q509.



Electron tunneling in tissue near SNc without ferritin, neuromelanin





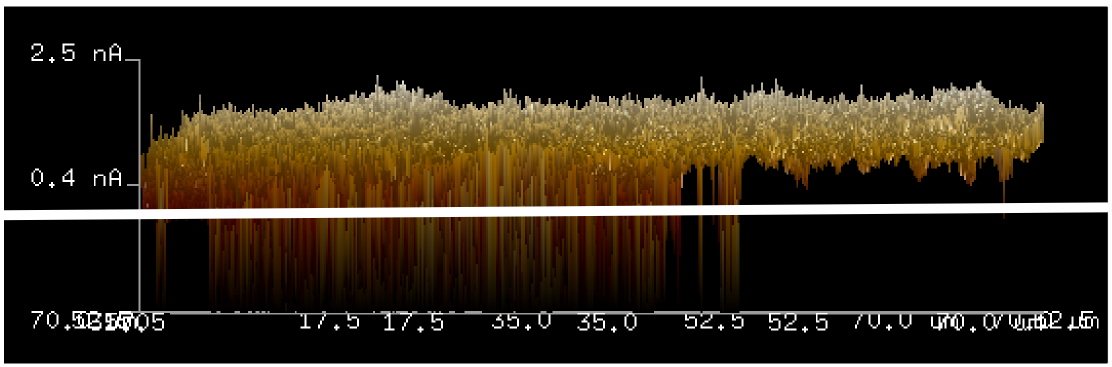


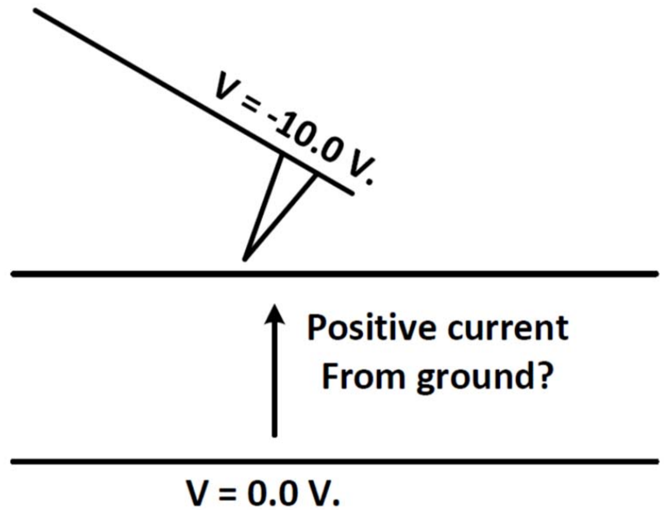
- **Conductive atomic force microscopy testing, -10 V bias on AFM nanoscale probe**
- **Negative currents to ground expected in control tissue**
- **Some areas provide insulation even with fields of 2 million volts per meter**

Rourk, Christopher J., Indication of quantum mechanical electron transport in human substantia nigra tissue from conductive atomic force microscopy analysis, *Biosystems* 179 (2019): 30-38.

~$4300

Electron tunneling in SNc tissue <u>with</u> ferritin, neuromelanin



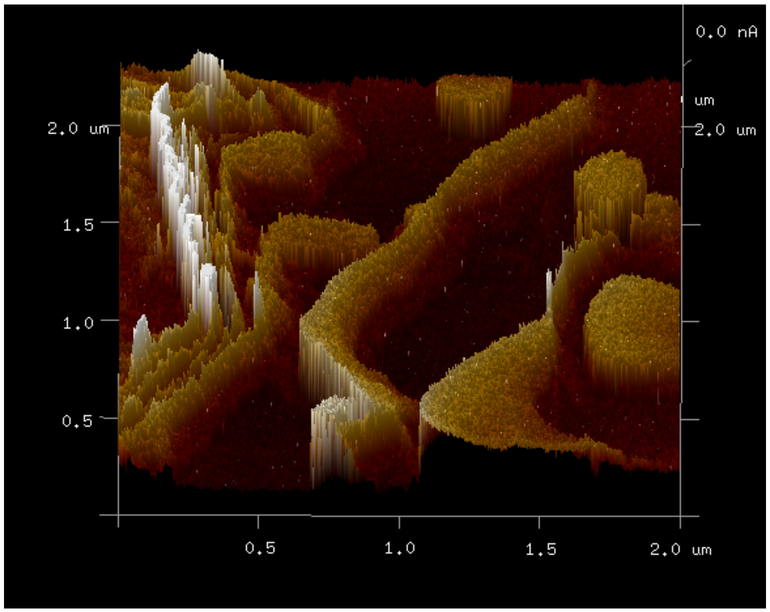


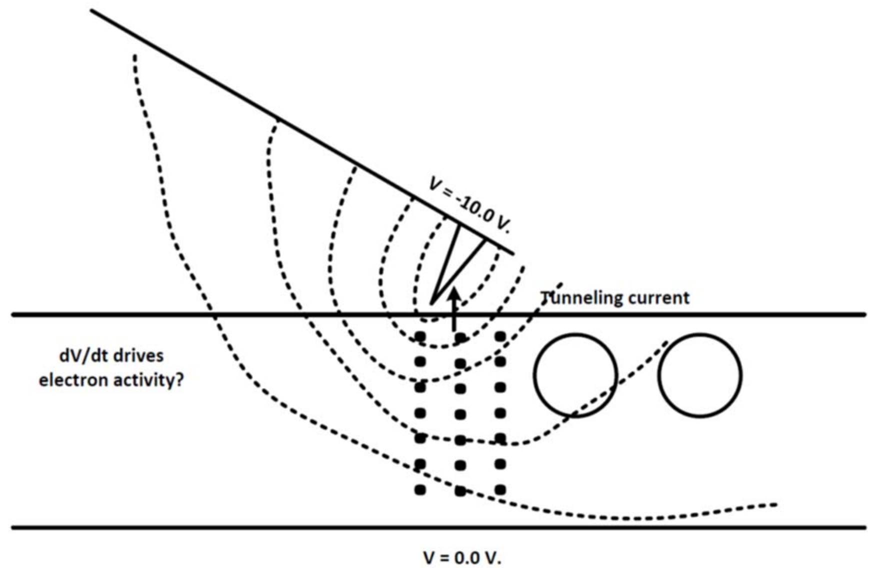
- **Conductive atomic force microscopy testing, -10 V bias on AFM probe**
- **Positive currents reflect electrons flowing into negative-biased AFM probe from grounded sample**
- **Electron tunneling can explain these measurements**

~$4300

Rourk, Christopher J., Indication of quantum mechanical electron transport in human substantia nigra tissue from conductive atomic force microscopy analysis, *Biosystems* 179 (2019): 30-38.

Electron tunneling in SNc tissue at higher resolution





- 2 micron x 2 micron resolution
- High currents correspond to dimensions of ferritin layers around neuromelanin organelles (NMOs)
- Electron movement driven by dV/dt?

~$4300

Rourk, Christopher J., Indication of quantum mechanical electron transport in human substantia nigra tissue from conductive atomic force microscopy analysis, *Biosystems* 179 (2019): 30-38.

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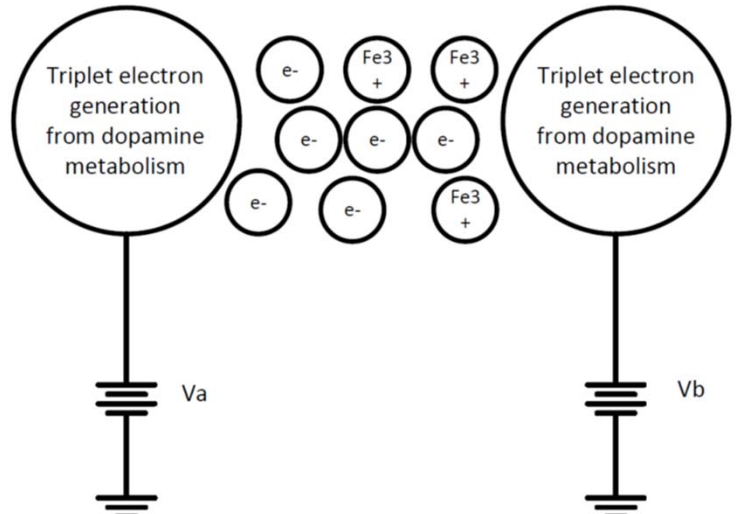
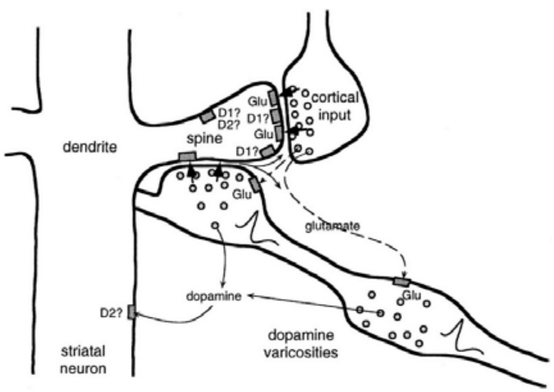
Tunneling between quantum dots causes the electron wave function to collapse

- “Although we prefer the amplitude point of view,(see B.Kayser and L. Stodolsky, Physics. Lett. B359 343 (1995)) one could also arrive at Eq (13) by ‘collapsing the wavefunction’ of the dot electron after every probing . . .” Stodolsky, L. "Measurement process in a variable-barrier system." Physics Letters B 459.1-3 (1999): 193-200.
- “The best answer, finally, to the ‘question of the collapse of the wavefunction’ is that there is no wavefunction.” Kayser, B., and L. Stodolsky, EPR experiments without ‘collapse of the wavefunction’. Physics Letters B 359.3-4 (1995): 343-350.

Modelling electron tunneling and electron wave function collapse in SNc ferritin



- Electron movement based on somatic dopamine metabolism, post-synaptic axon activity from cortical neurons.



"Dopamine neurons are activated by rewarding events that are better than predicted, remain uninfluenced by events that are as good as predicted, and are depressed by events that are worse than predicted."

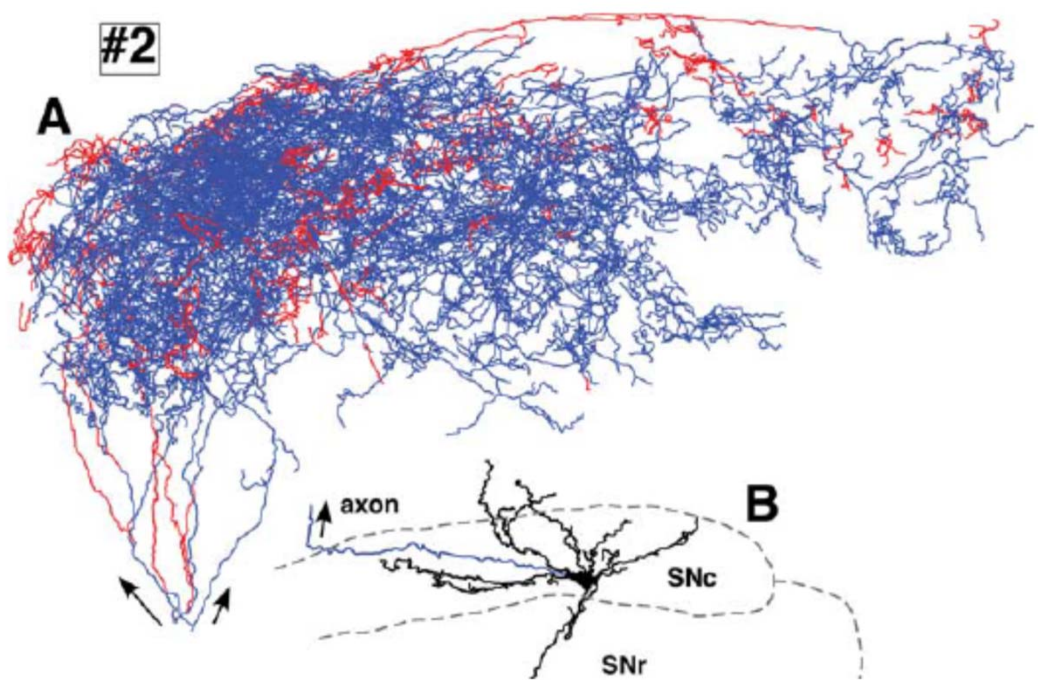
For movement control, dopamine modulates moment-by-moment activity in the striatum to mediate action selection.

Liu, Changliang, Pragya Goel, and Pascal S. Kaeser. "Spatial and temporal scales of dopamine transmission." *Nature Reviews Neuroscience* 22.6 (2021): 345-358.

Schultz, Wolfram. "Predictive reward signal of dopamine neurons." *Journal of neurophysiology* 80.1 (1998): 1-27.

Large SNc dopamine neurons

- Extensive axonal arbors (most SNc neurons are small)
- Connect to cortical axons at striatal dendrites, which cause SNc neurons to fire
- Mechanism needed to prevent conflicts/seizures
- Could integrate cortical signals when no action is being selected



Matsuda, Wakoto, et al. "Single nigrostriatal dopaminergic neurons form widely spread and highly dense axonal arborizations in the neostriatum." *Journal of Neuroscience* 29.2 (2009): 444-453.

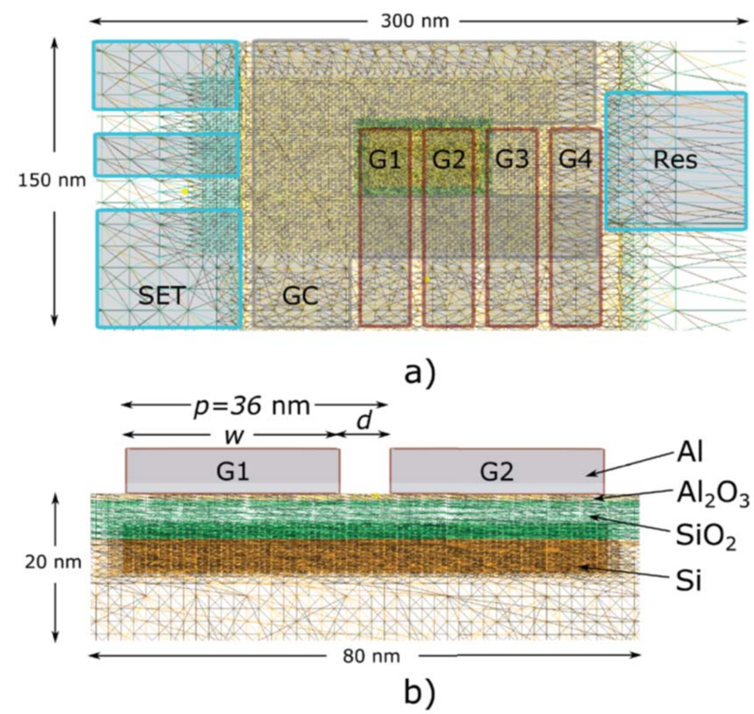
Modeling electron tunneling in ferritin – PYXIAD (Python EXtension for Ab Initio Dynamics)

- "Well separated energy levels and localized states suggest that decoherence effects should be taken into account. This situation is very common for molecules, quantum-confined systems (e.g., quantum dots, nanotubes), and some condensed matter materials. . . .**Decoherence causes the electronic wave function to collapse to adiabatic states**."
- May be limited to several hundred atoms.
- Magnon/electron spin modeling capability unclear.

Akimov, Alexey V., and Oleg V. Prezhdo. "Advanced capabilities of the PYXAID program: integration schemes, decoherence effects, multiexcitonic states, and field-matter interaction." *Journal of chemical theory and computation* 10.2 (2014): 789-804.

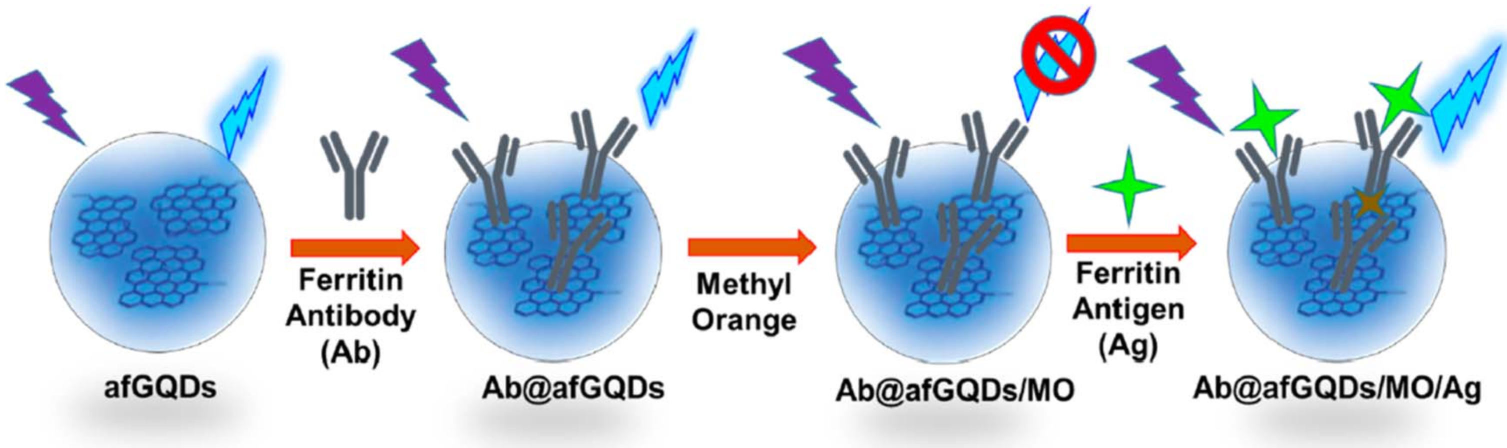
Modeling electron tunneling in ferritin – NEMO5

- Single electron transistor (“SET”) - Coulomb blockade used for selective tunneling of a up or down spin electron from/to dots G1-G4.
- The mesh has ~ 550, 000 nodes and ~ 3.5 million elements.
- Simple model of SNc transport possible?



Sahasrabudhe, Harshad. *Low Temperature Simulations Framework for Quantum Dots and Point Contacts*. Diss. Purdue University, 2018.

Measuring electron tunneling in ferritin



- QD fluorophores tagged to ferritin can potentially be used to detect tunneling (instead of UV excitation source).
- Similar to mechanism used to generate photons in QD LEDs.

Garg, Mayank, et al. "Amine-Functionalized Graphene Quantum Dots for Fluorescence-Based Immunosensing of Ferritin." *ACS Applied Nano Materials* 4.7 (2021): 7416-7425.

Summary

- Ferritin supports coherent electron tunneling.
- Each tunneling event corresponds to a collapse event.
- Electron transport between large SNc neurons through ferritin arrays, and associated wave function collapse, could be modeled and tested.

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Ms. Betony Adams, University of KwaZulu-Natal

Prof. Doug Brash, Yale

Prof. Sierin Lim, National Technological University of Singapore

Prof. Olivier Pluchery, Sorbonne University

Dr. Olga Mykhailyk, ethris GmbH

Prof. Heinz Nakotte, New Mexico State University

Prof. Ilya Bezprozvanny, U.T. Southwestern

Prof. Dwight German, U.T. Southwestern

Prof. Majid Minary, Arizona State University

Prof. Igamberdiev, Memorial University