GOLD NANOCLUSTER SENSOR SIGNALS OF DOPAMINE WITH TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

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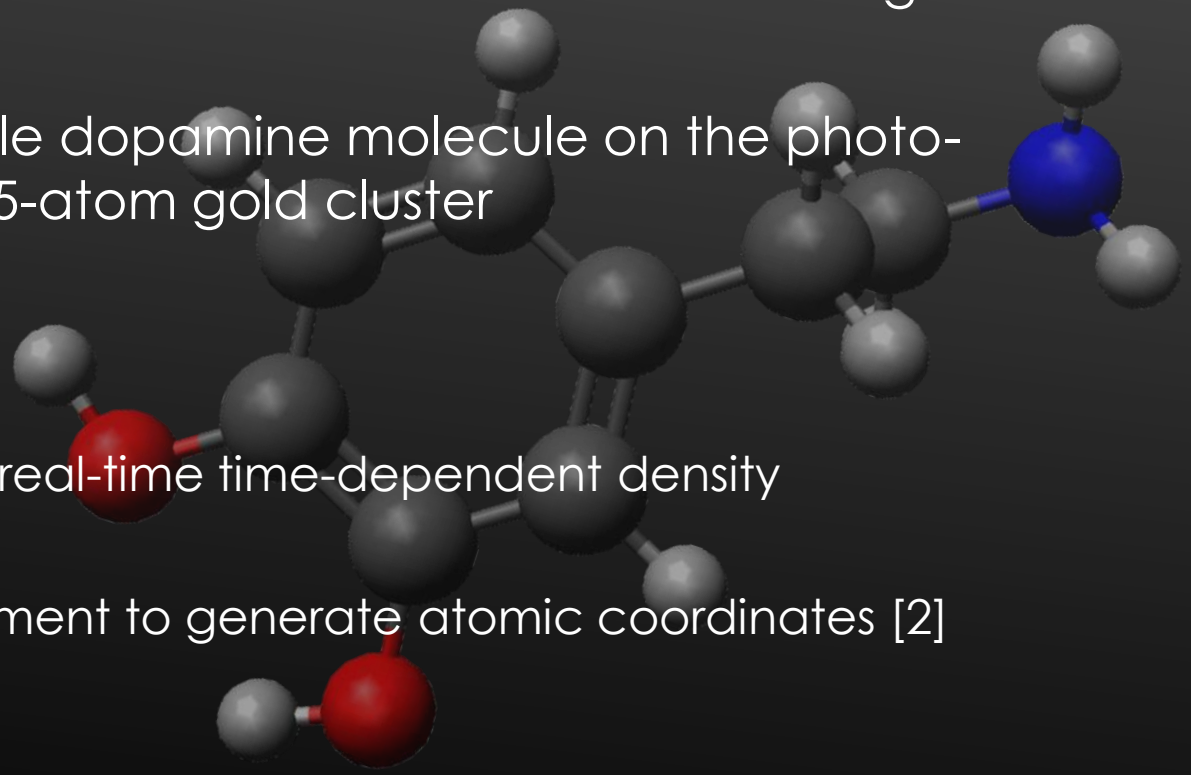
AIMS AND MOTIVATION

- Use computational approaches to model the detection of single dopamine molecules
- Analyse the effect of a single dopamine molecule on the photo-absorption spectrum of a 55-atom gold cluster



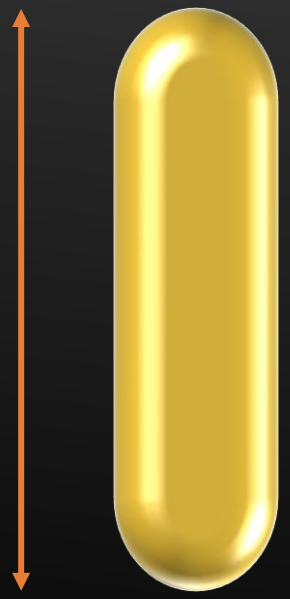
- Software:
  - GPAW implementation of real-time time-dependent density functional theory [1]
  - Atomic simulation environment to generate atomic coordinates [2]

[1] J Enkovaara *et al* 2010 *J. Phys.: Condens. Matter* **22** 253202
[2] Ask Hjorth Larsen *et al* 2017 *J. Phys.: Condens. Matter* **29** 273002

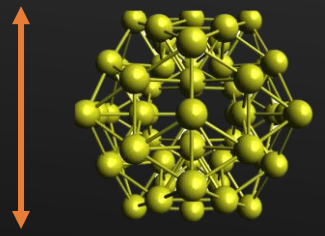
NANOPARTICLE VS ATOMIC-SIZED CLUSTER

- Classical Mie theory description for nanoparticle vs quantum description for atomic-sized cluster
- Nanocluster has more molecule-like optical properties

< 100 nm
A few thousand atoms

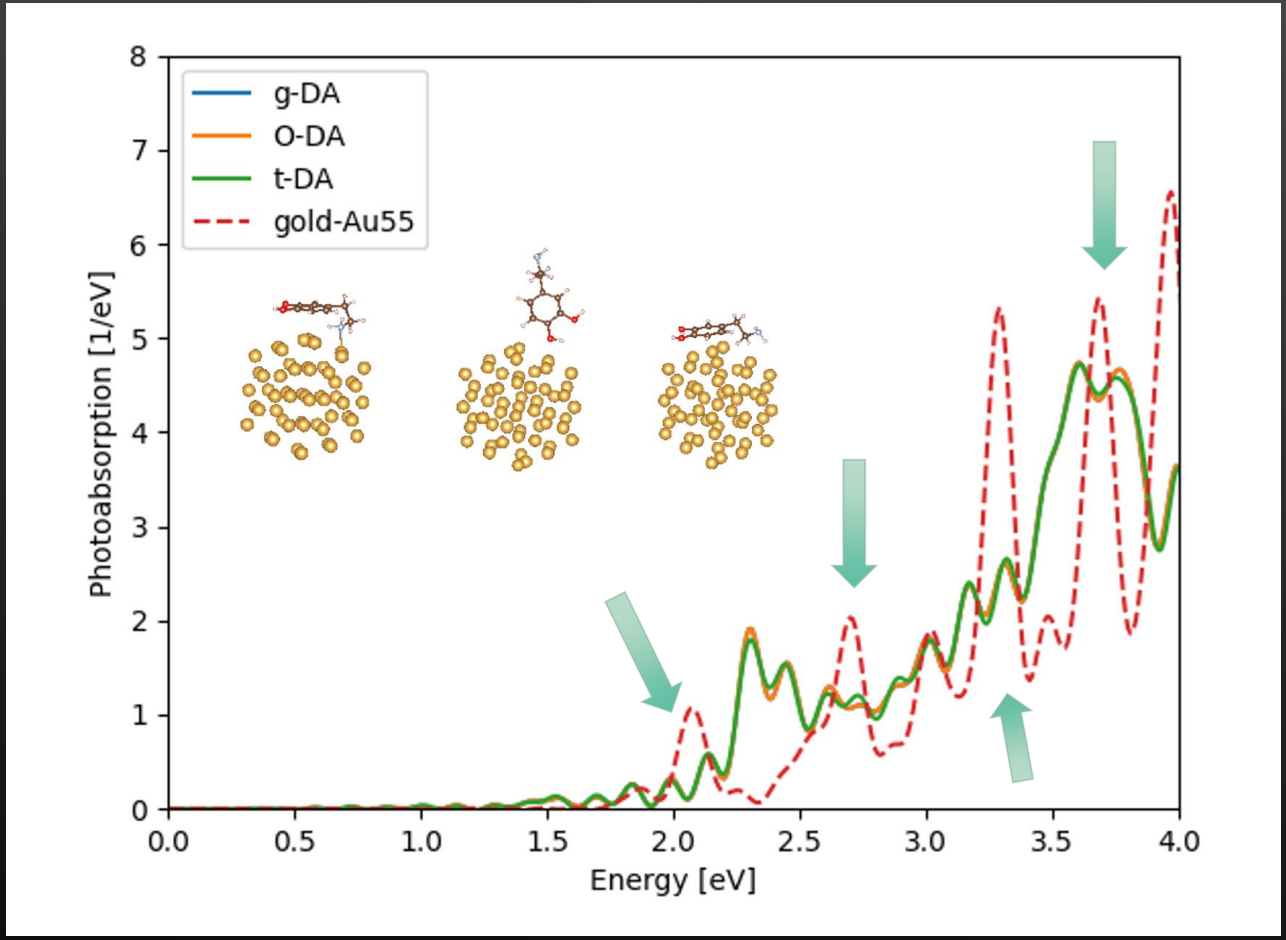


< 2 nm
Less than a few hundred atoms



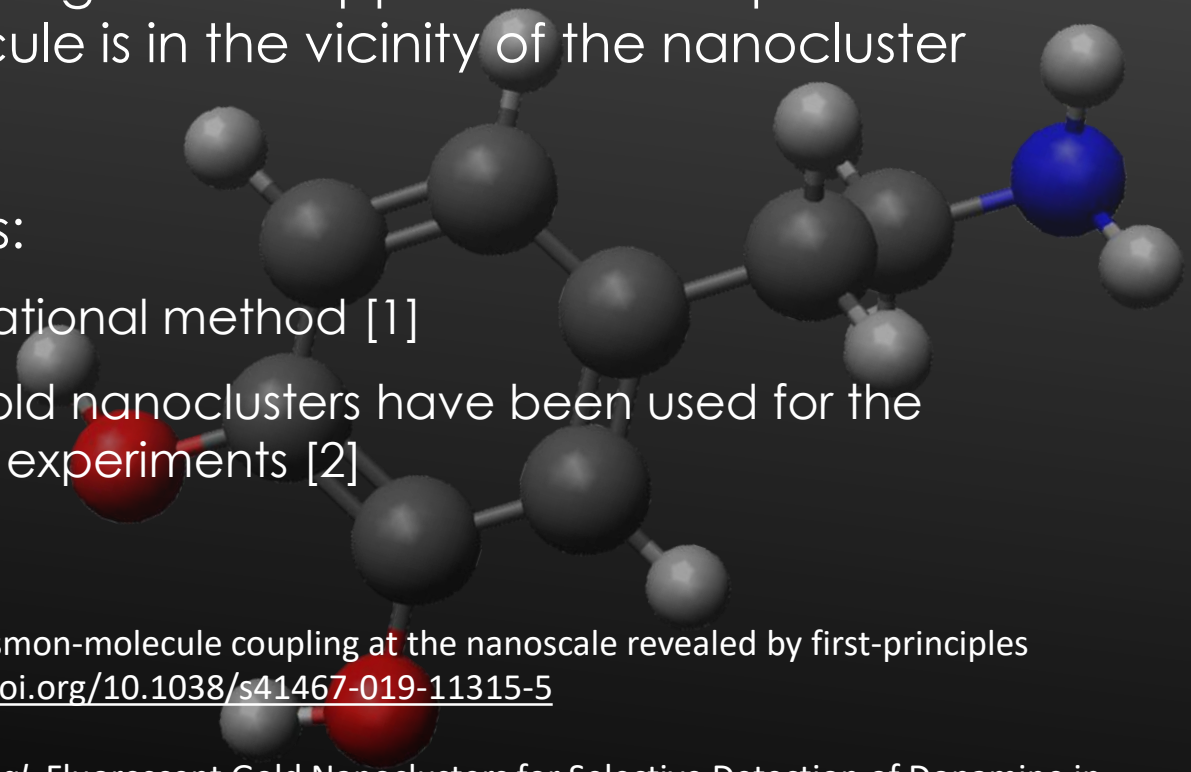
RESULTS

- Optical properties shown for the visible to UV range
- Different orientations of dopamine produce the same photo-absorption spectrum
- Evidence of multiple Rabi splitting for the gold peaks
- However, the intensity of the signals is rather weak



STRONG COUPLING

- Gold absorption peaks splitting into an upper and lower polariton when the dopamine molecule is in the vicinity of the nanocluster



- Outlook and considerations:
  - Benchmarking of computational method [1]
  - Functionalized 30-atom gold nanoclusters have been used for the detection of dopamine in experiments [2]

[1] Rossi, T.P., Shegai, T., Erhart, P. *et al.* Strong plasmon-molecule coupling at the nanoscale revealed by first-principles modeling. *Nat Commun* **10,** 3336 (2019). https://doi.org/10.1038/s41467-019-11315-5

[2] Govindaraju, S., Ankireddy, S., Viswanath, B. *et al.* Fluorescent Gold Nanoclusters for Selective Detection of Dopamine in Cerebrospinal fluid. *Sci Rep* **7,** 40298 (2017). https://doi.org/10.1038/srep40298

SUMMARY

- The main features of the photo-absorption spectrum are reliably reproducible for different orientations of dopamine on the gold cluster
- These results provide a starting point to map first principles calculations to experimental data for the detection of dopamine with atomic-sized gold clusters