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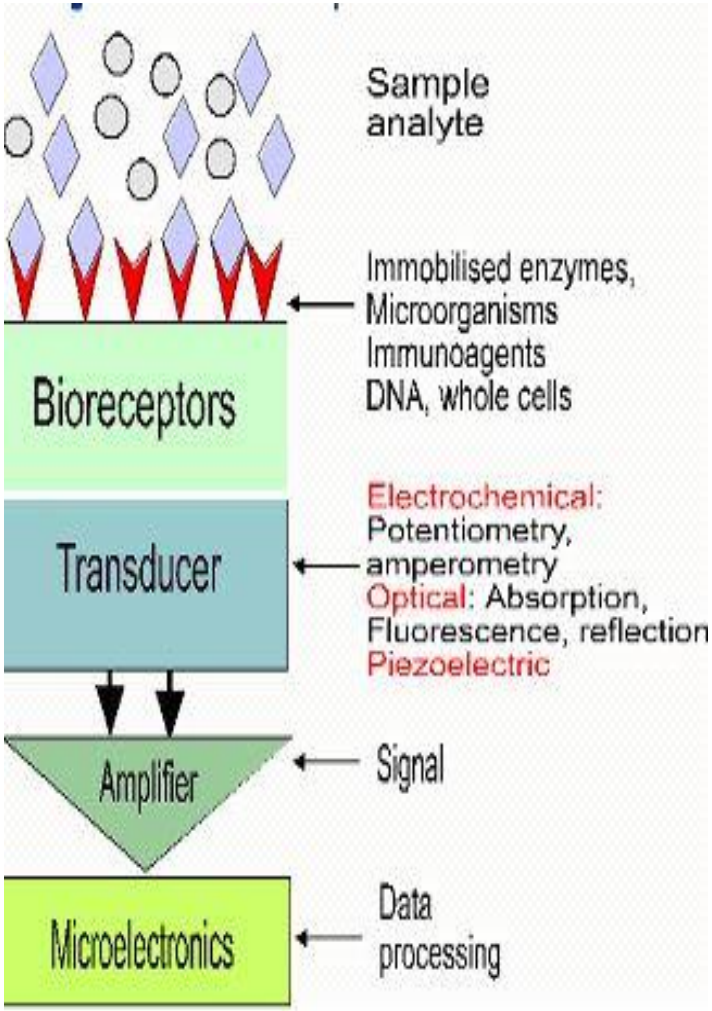
Understanding the Role of Nanomaterials in DNA Biosensors Through Finite Element Analysis

J. Carl Kumaradas, Anthony Zhang, and
Yevgeniy D. Davletshin
Toronto, Ontario.
ckumarad@ryerson.ca

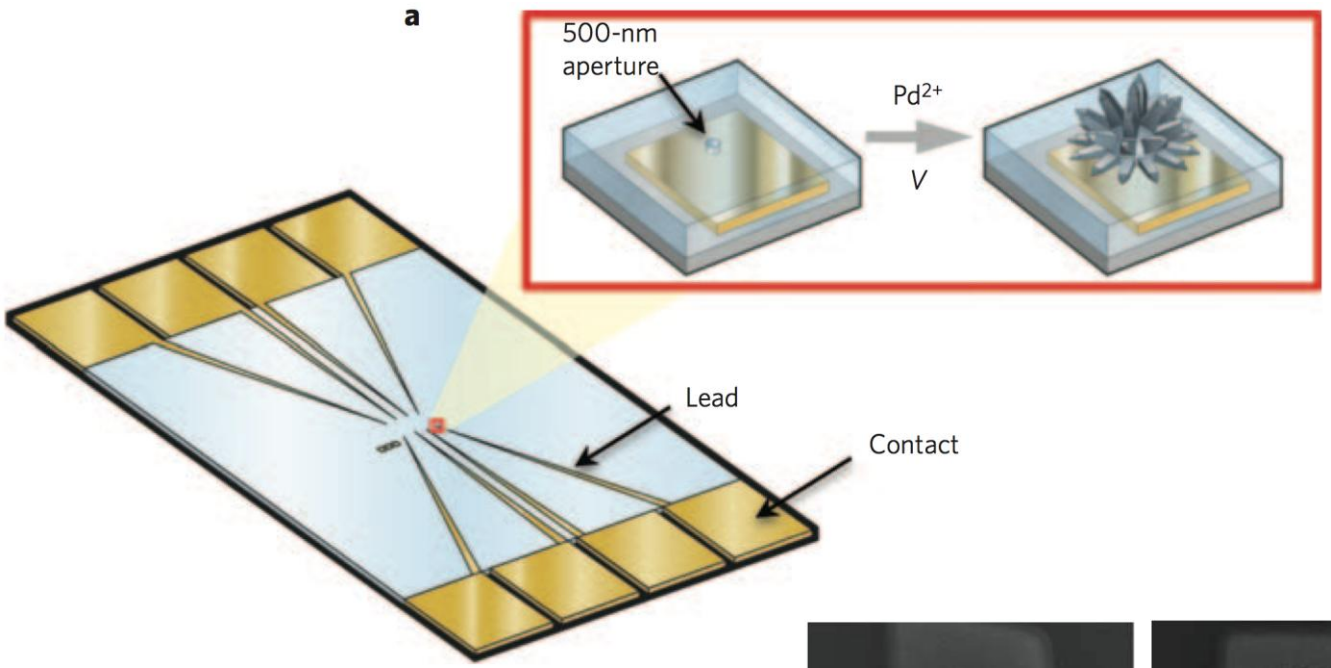
What are biosensors?

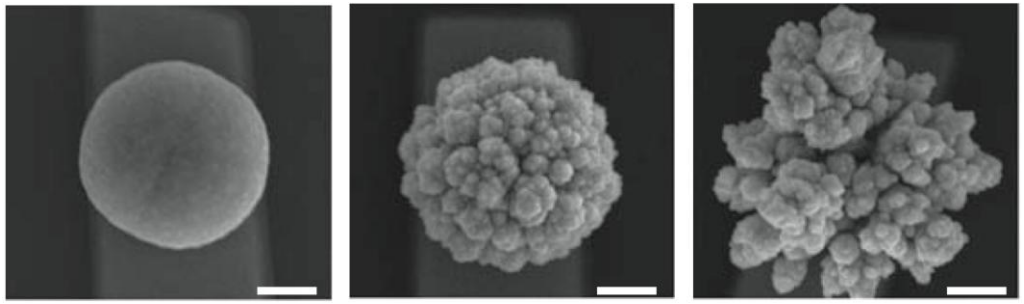
- Determines the presence or detects the concentration of a target molecule in a solution
- Practical uses in medicine, biology, food quality etc.



Campanella, L. (2005). Sensitized Biosensors for Protection of the Atmosphere and the Human Health. Retrieved August 2, 2011.

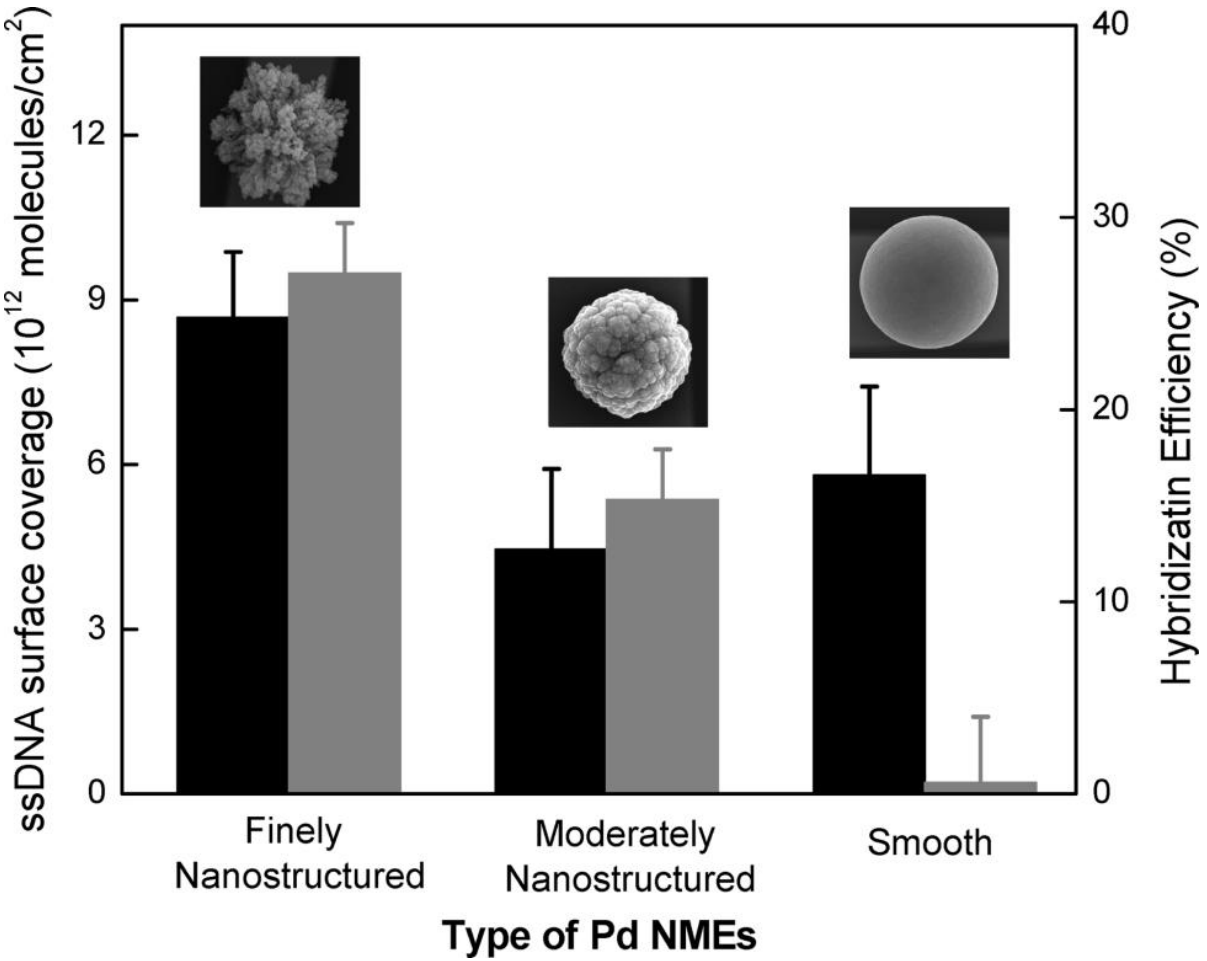
Nano structured probes





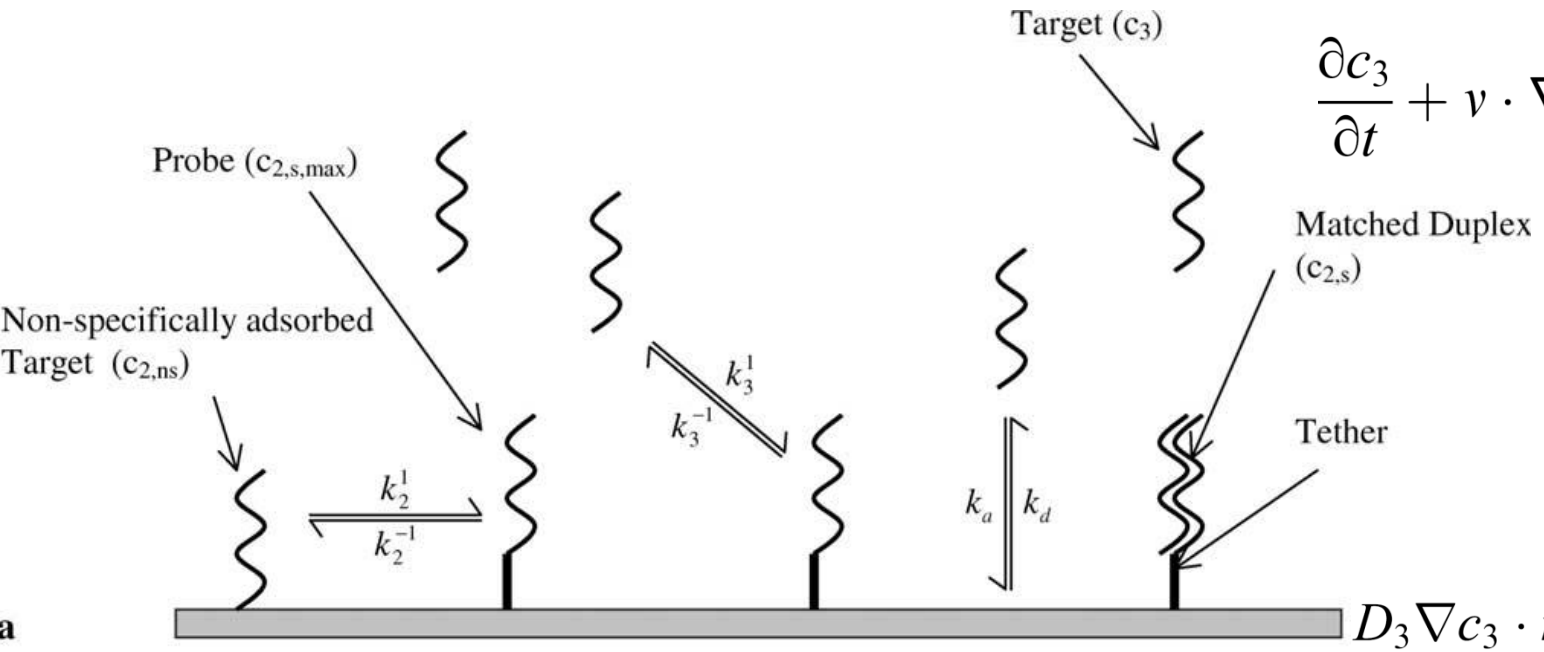
Soleymani, L., Fang, Z., Sargent, E. H., & Kelley, S. O. (2009). *Nature nanotechnology*, 4(12), 844–8.

DNA hybridization efficiency of nano-structured surfaces



Bin, X., Sargent, E. H., & Kelley, S. O. (2010). *Analytical Chemistry*, 82(14), 5928–5931.

Physics of bulk and surface phases



$$\frac{\partial c_3}{\partial t} + v \cdot \nabla c_3 = D_3 \nabla^2 c_3$$

$$D_3 \nabla c_3 \cdot n = \frac{\partial c_{2,s}}{\partial t} + \frac{\partial c_{2,ns}}{\partial t}$$

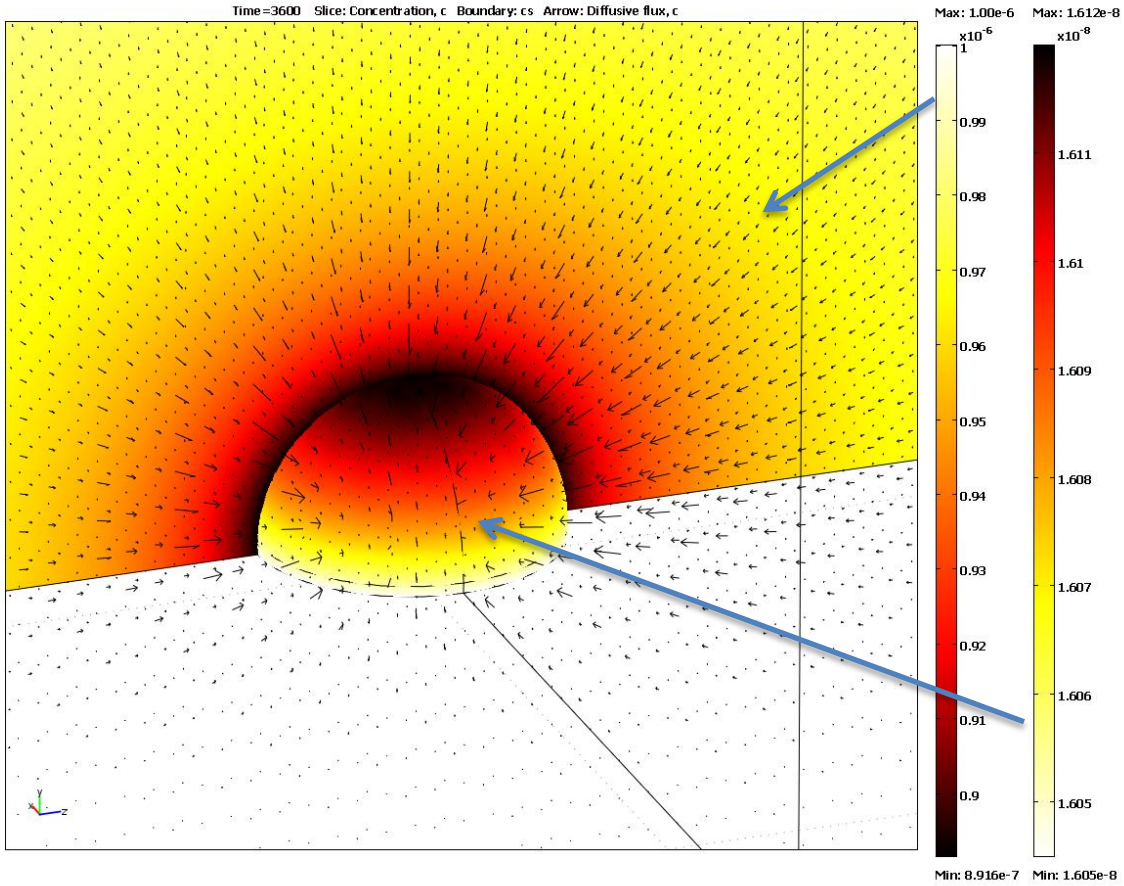
$$\frac{\partial c_{2,s}}{\partial t} = \left[k_3^1 c_{3,m}(c_{2,s,max} - c_{2,s}) - k_3^{-1} c_{2,s}\right] + \left[k_2^1 c_{2,ns}(c_{2,s,max} - c_{2,s}) - k_2^{-1} c_{2,s}\right],$$

$$\frac{\partial c_{2,ns}}{\partial t} = \left[D_2 \nabla^2 c_{2,ns}\right] + \left[k_a c_{3,m}(c_{2,ns,max} - c_{2,ns}) - k_d c_{2,ns}\right] - \left[k_2^1 c_{2,ns}(c_{2,s,max} - c_{2,s}) - k_2^{-1} c_{2,s}\right],$$

Erickson, D., Li, D., & Krull, U. J. (2003). Analytical Biochemistry, 317(2), 186–200.

Surface hybridizaton concentration and bulk analyte concentration

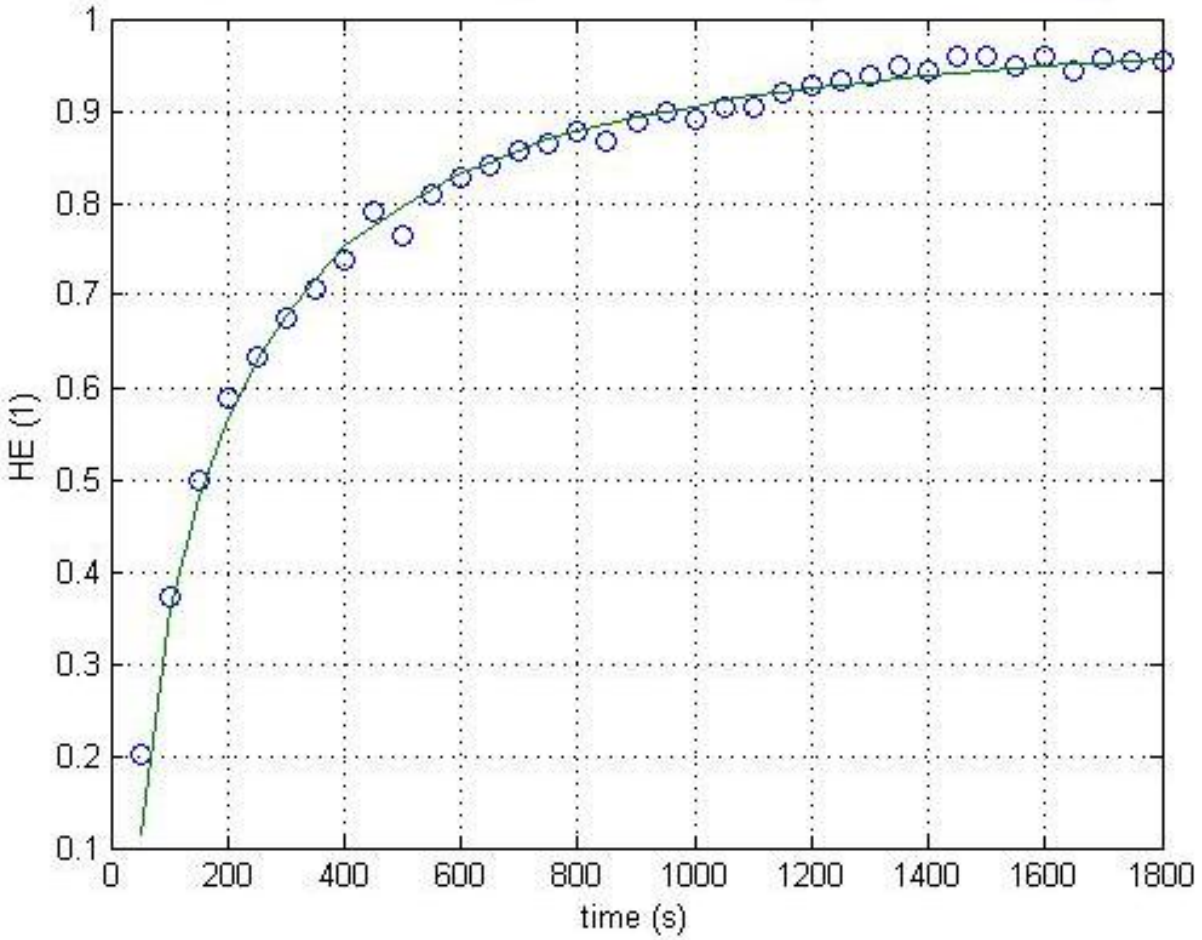
- Materials
- Transport of Diluted Species *(chds*
  - Diffusion
  - No Flux
  - Initial Solution Concentration
  - Periodic Condition X
  - Periodic Condition Y
  - Outer Boundary Concentration
  - Surface Outflow
- Sensor Surface PDE *(c_2_s)*
  - Weak Form PDE 1
  - Initial Surface Concentration
  - Weak Form PDE 2
  - HE Equation
- Sensor Base PDE *(c_2_ns)*
  - Weak Form PDE 1
  - Initial Base Concentration
  - Weak Form PDE 2



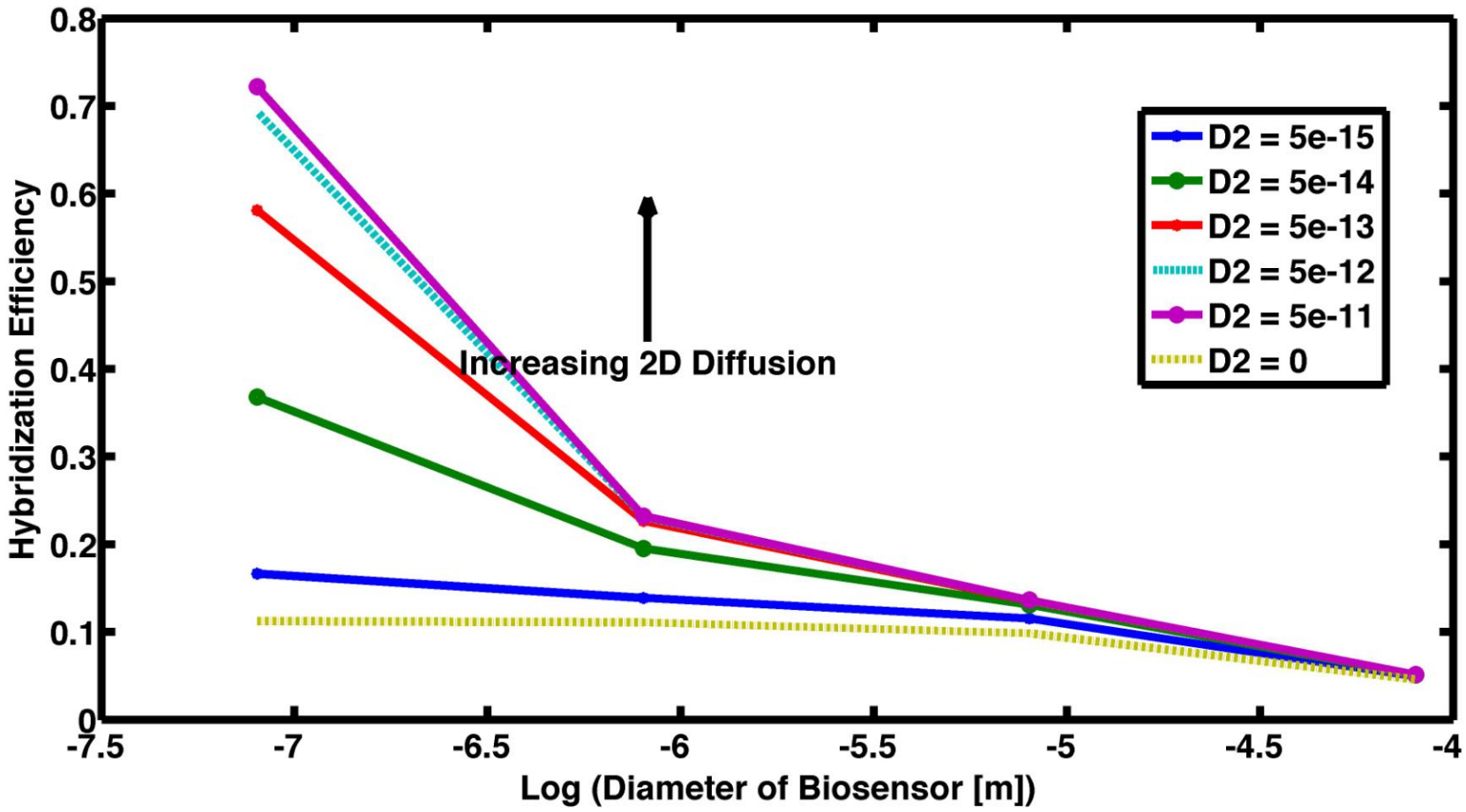
$$HE = \frac{\int_S c_{2,s}\, ds}{\int_S c_{2,s,\max}\, ds}$$

Verification / fit to experiment

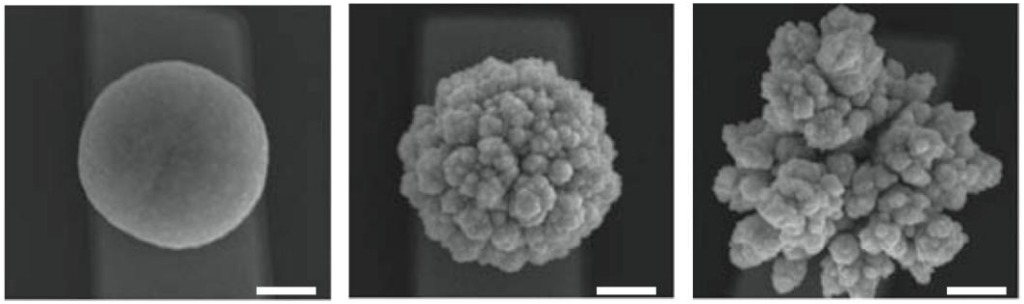
Experimental data from Peterson, A. W., Heaton, R. J., & Georgiadis, R. M., *Nucleic Acids Research*, 29(24), 5163–5168, 2001.

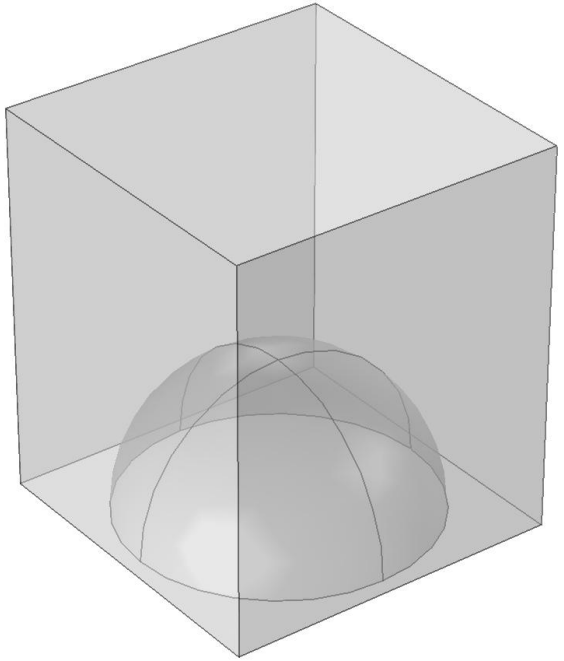


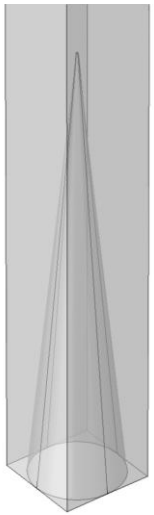
Role of biosensor size



Resolving the nano-structure







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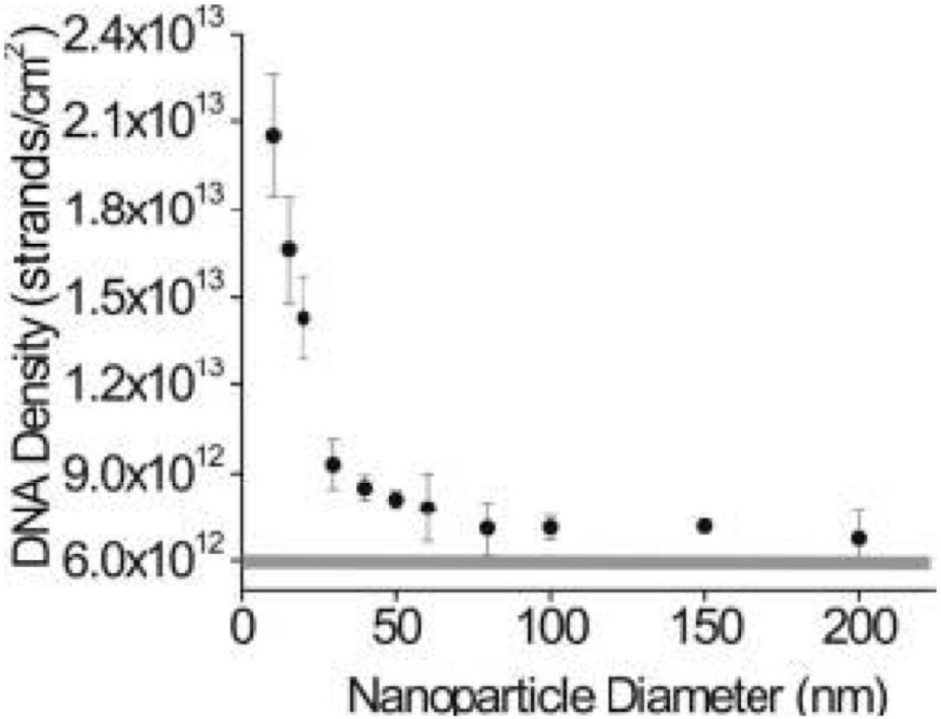
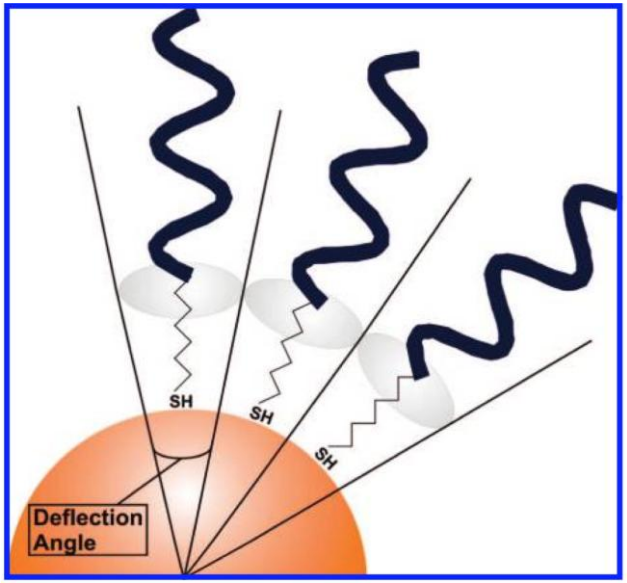
Role of curvature in reactions





Hill, H. D., Millstone, J. E., Banholzer, M. J., & Mirkin, C. a. (2009). *ACS nano*, 3(2), 418–24.

Conclusions and future work

- Surface hybridization successfully modeled smooth surfaces.
- Role of nano-structuring not clear.
- Consider rate constants as a function of radius of curvature of nano-structures.
- Investigate role of surface diffusion on nano-structured surfaces.

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