Controlling surface-enhanced charge screening to realize single-molecule sensing with silicon FET sensors

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1. Introduction

Large-scale single-molecule sensing to enable & boost applications in the life sciences (e.g. SMRT sequencing)

Silicon **Field-Effect Transistor (FET) sensor**:

- Real-time **charge-based sensing** of biomolecules and/or ions
- Paragon of **embeddable & scalable** technology

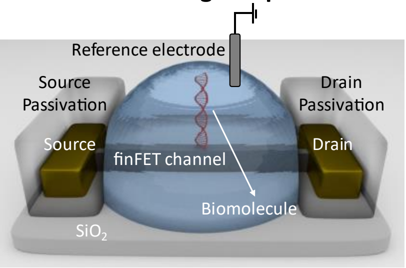
→ **Unprecedented troughput & parallelism**

No single-molecule detection achieved

Main **sensitivity-limiting** factor is electrolyte **charge screening**

- Enhanced by charged and pH-sensitive oxide surface sites

  → **non-linear screening** and **pH feedback effect**



2. FET sensor modeling

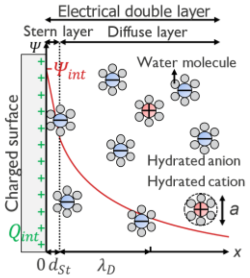
a. Non-linear screening

- Formation of **electrical double layer** at charged entity: screening by near-exponential distribution of ions
- **Increased ion concentration** ($c_\pm$) in diffuse layer **enhances** electrolyte **screening**

Bikerman model:

$$c_\pm = \frac{c_0 \exp\left(\frac{\mp q\psi}{kT}\right)}{1 + 4a^3 {c_0}^2 \sinh^2\left(\frac{q\psi}{2kT}\right)}$$

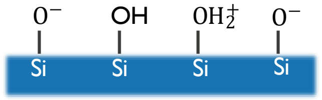
c_0 is bulk ion conc.



b. pH feedback effect

- **Biomolecule charge alters local** proton conc. $[H^+]_{int}$ or **pH** at the FET surface
- **pH-sensitive** oxide surface **sites** induce a **counter charge**

$$-SiO^- \underset{H^+}{\overset{K_a}{\rightleftharpoons}} -SiOH \underset{H^+}{\overset{K_b}{\rightleftharpoons}} -SiOH_2^+$$



For SiO_2:

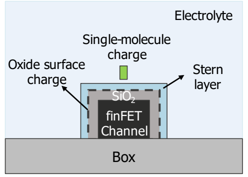
$$K_a = \frac{[H^+]_{int}\Gamma_{SiO^-}}{\Gamma_{SiOH}} \qquad pK_a = 4.5$$

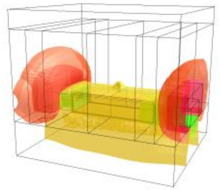
$$N_t = \Gamma_{SiOH} + \Gamma_{SiO^-} = 4 \times 10^{13}\ cm^{-2}$$

3. Single-molecule TCAD simulation

a. finFET with discrete biomolecule

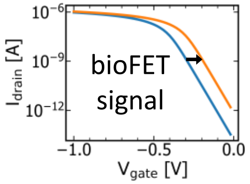
- 15bp dsDNA = 30 charges
- 1.5 mM salinity and pH 7





b. Simulation of single-molecule SNR

- **Signal** is ΔV_g of I_d-V_g curve due to charge of biomolecule
- **Noise** is $\Delta V_{trap}\sqrt{D_{trap}A_{eff}}$



D_{trap} = Calibr. oxide trap density

A_{eff} = effective FET surface area

4. Results and discussion

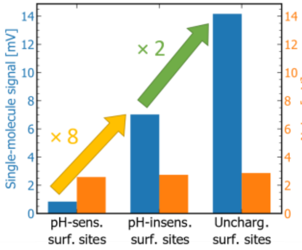
pH-insensitive surface sites

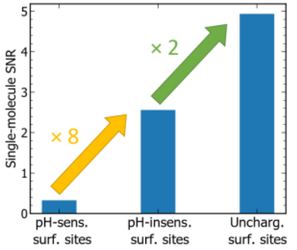
- **8x boost** in signal and SNR

Uncharged surface sites

- Extra **2x boost** in signal and SNR

Noise unaffected





To **boost FET single-molecule sensitivity**, one must select a gate oxide with **lowly-charged** and **pH-insensitive** surface sites