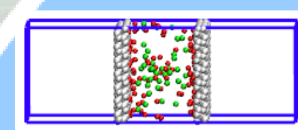
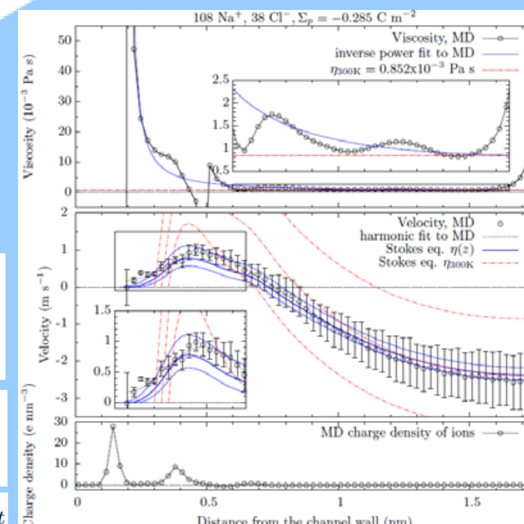
Surface charge effects on the nano-electro-osmosis

Bohumir Jelinek

Postdoctoral Fellow

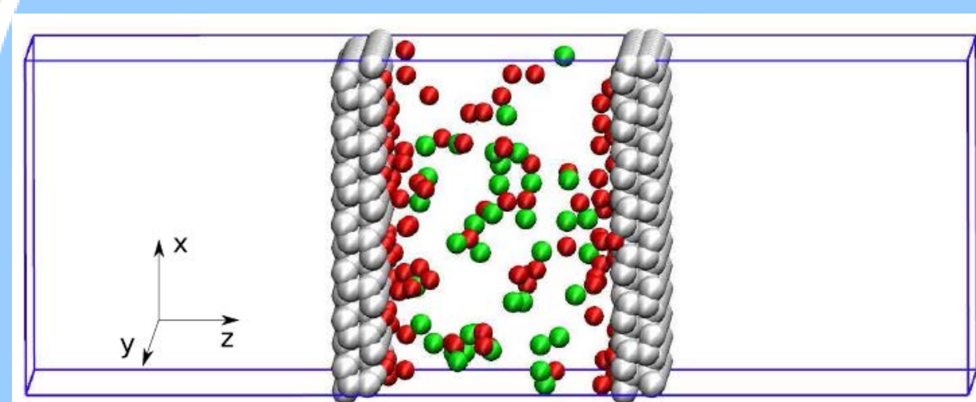
CAVS, Mississippi State University





$$\frac{d}{dz}\left[\eta(z)\frac{du_x(z)}{dz}\right] = -F_d(z)$$

$$\mathbf{F}_d(z) = e\left[c_{\mathrm{Na}^+}(z) - c_{\mathrm{Cl}^-}(z)\right]\mathbf{E}_{ext}$$



Columbus, 11/27/2012

US Army Corps of Engineers

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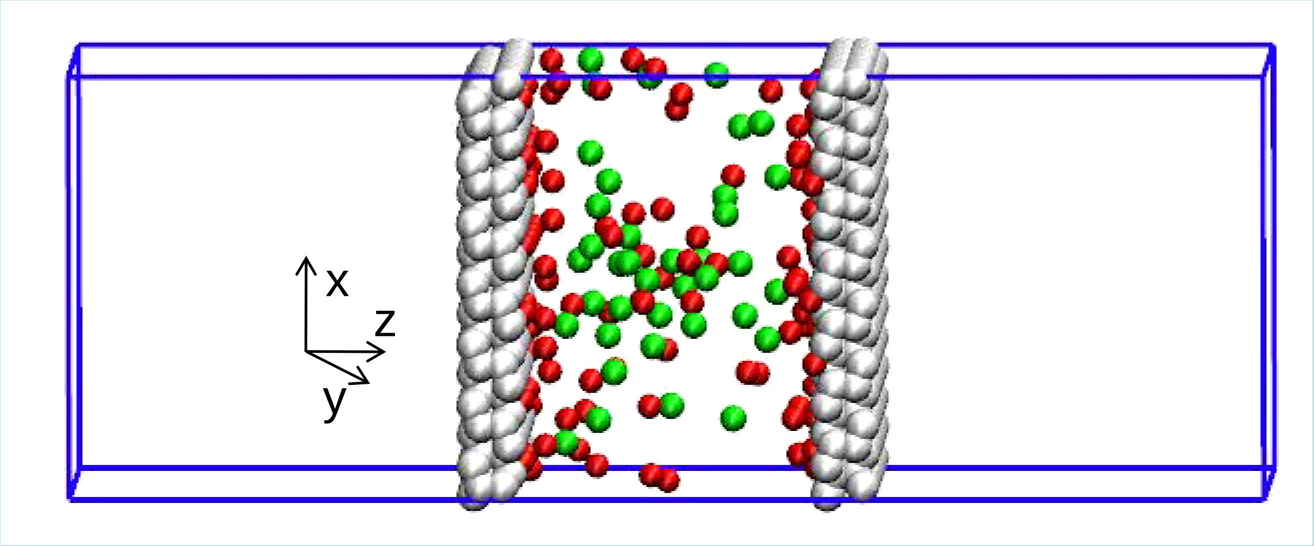
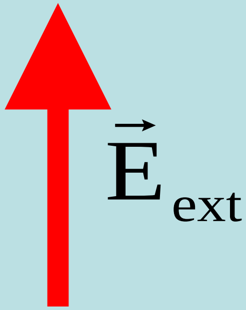
Electro-osmotic flow model





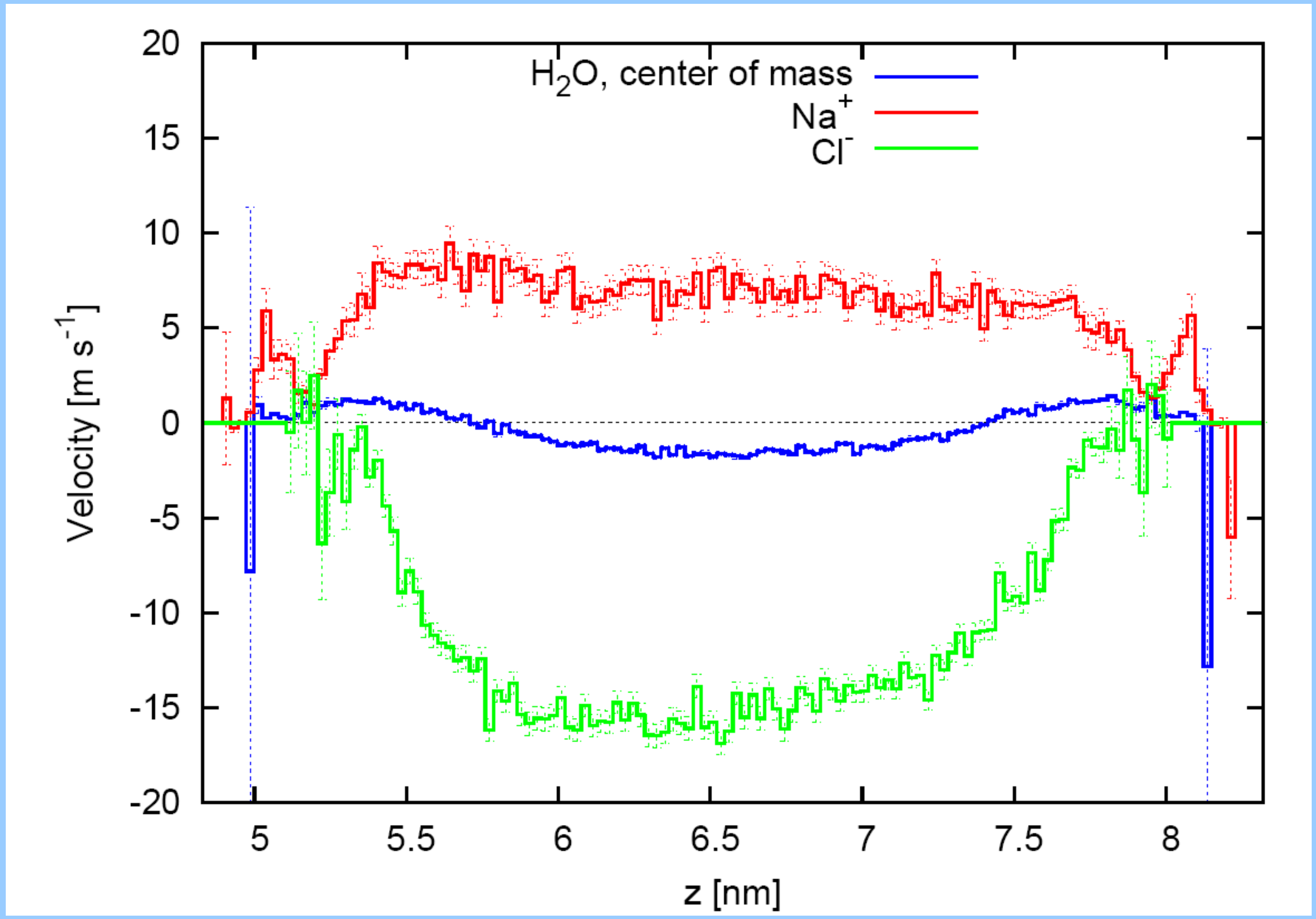
Fixed Si channel walls, innermost layer charged negatively

Dimensions of a solute region 4.66x4.22x3.49 nm, PBC x,y.

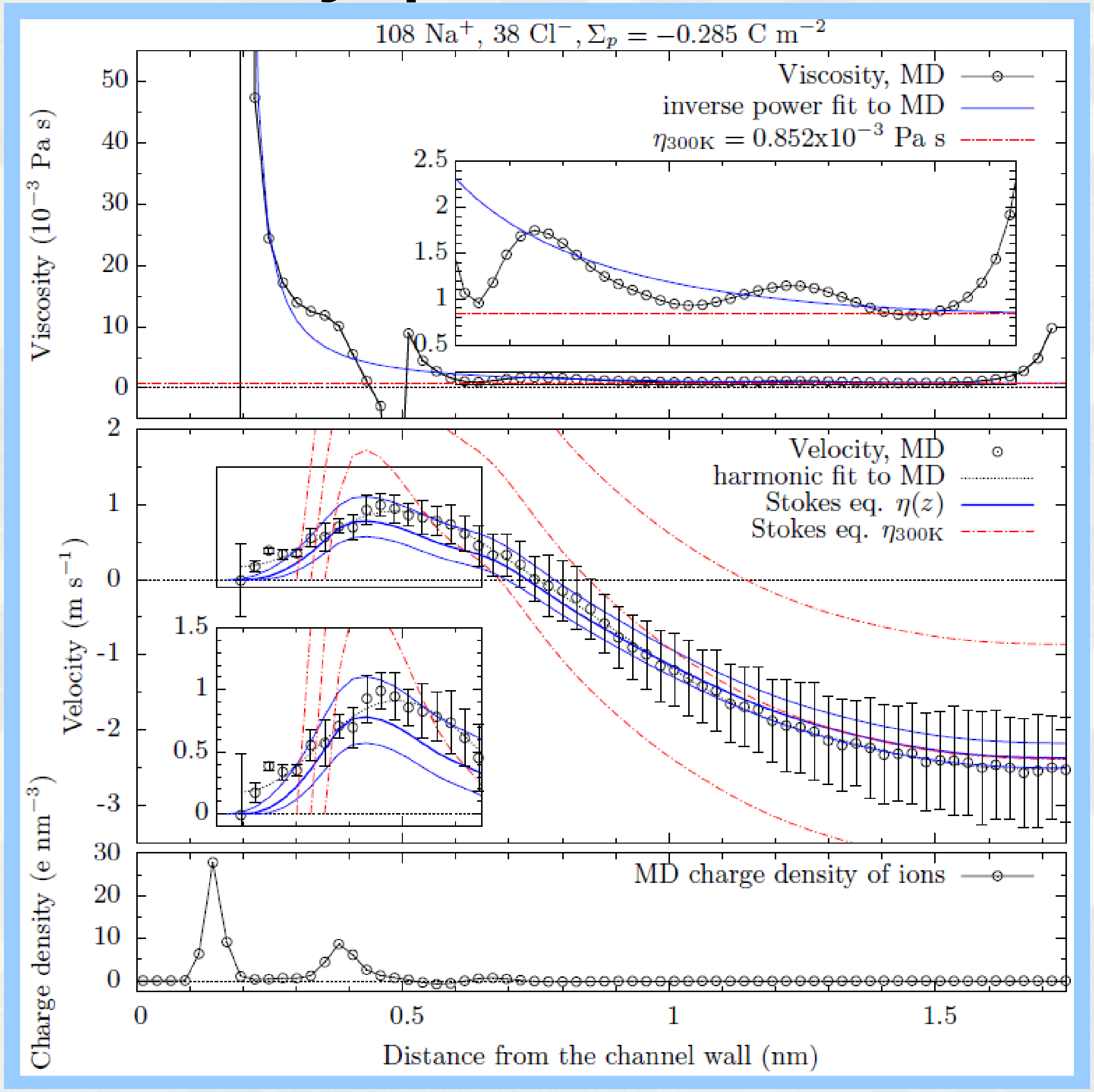
108 Na^+, 38 Cl^-, 2144 SPC/E H_2O molecules (not shown)

R. Qiao and N. R. Aluru: Charge Inversion and Flow Reversal in a Nanochannel Electro-osmotic Flow, PRL 92 (19) 2004

Velocity profiles



Velocity predicted from charge density



Stokes equation:

$$\frac{d}{dz}\left[\eta(z)\frac{du_x(z)}{dz}\right] = -F_d(z)$$

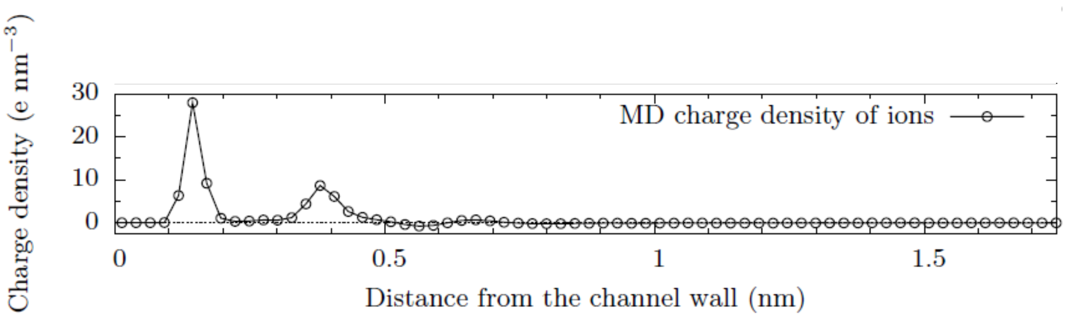
Blue:
inverse power viscosity

$$\eta(z) = \left[1 - \left(\frac{z}{h}\right)^2\right]^{-p} \eta_{\exp}$$

Red:
constant viscosity

Black circles:
Molecular Dynamics

Velocity predicted from charge density



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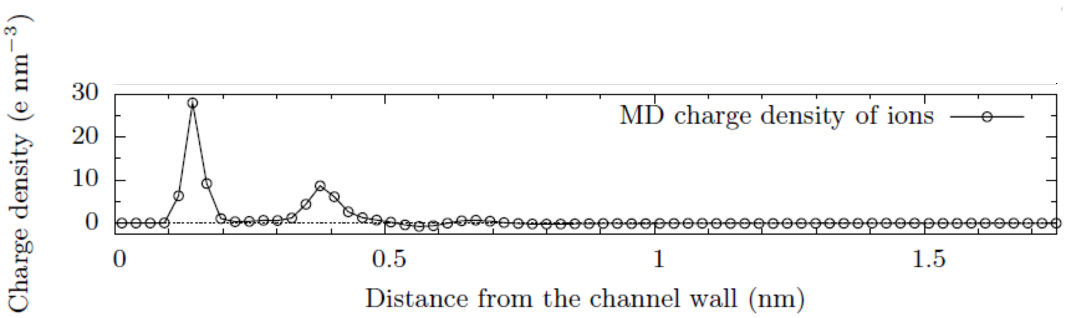

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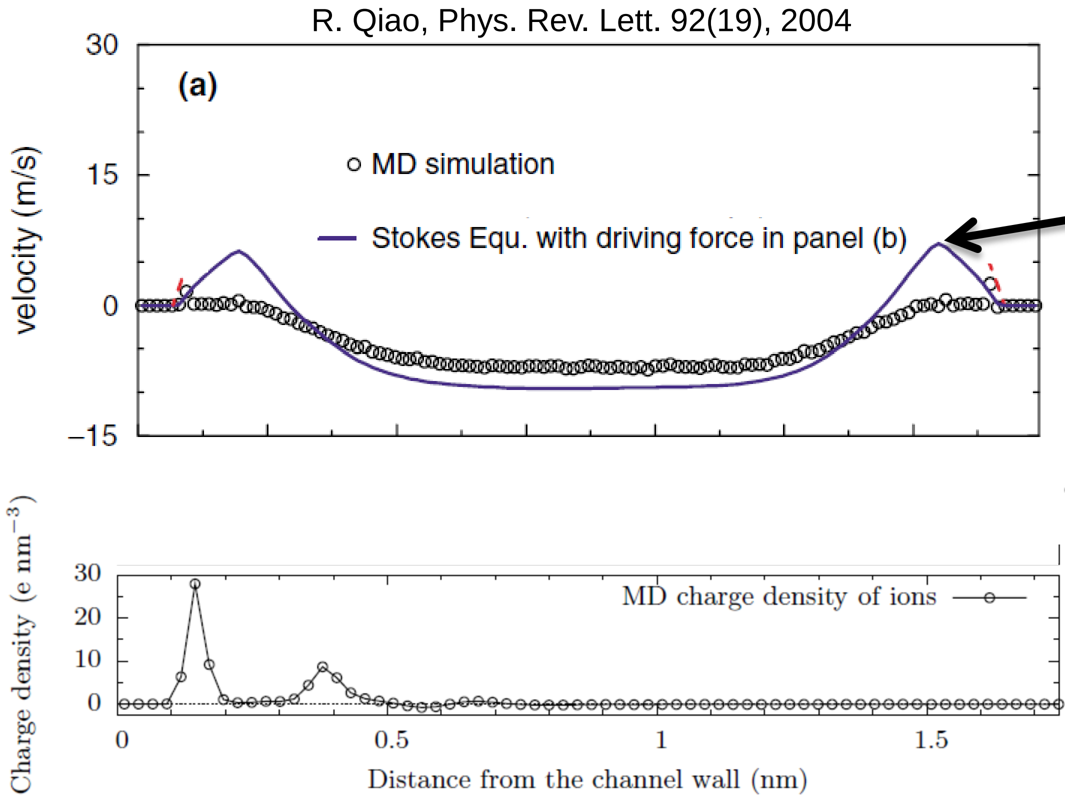

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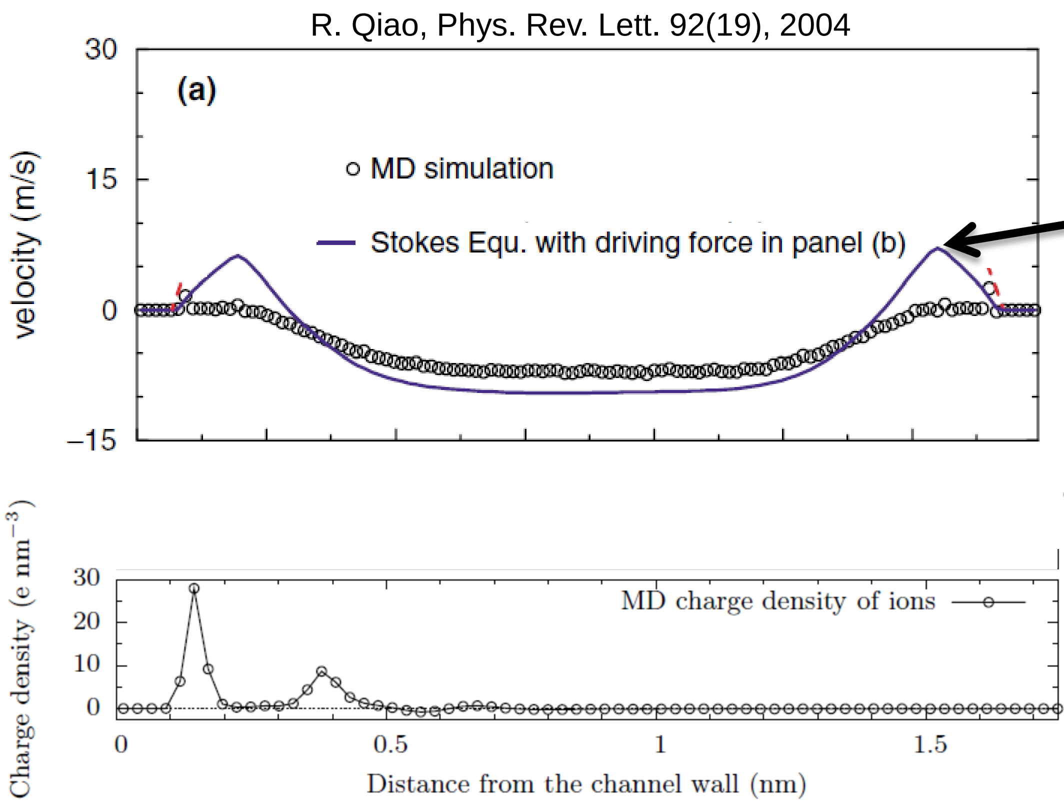
Dark blue line:
velocity prediction
from MD charge density

Velocity predicted from charge density

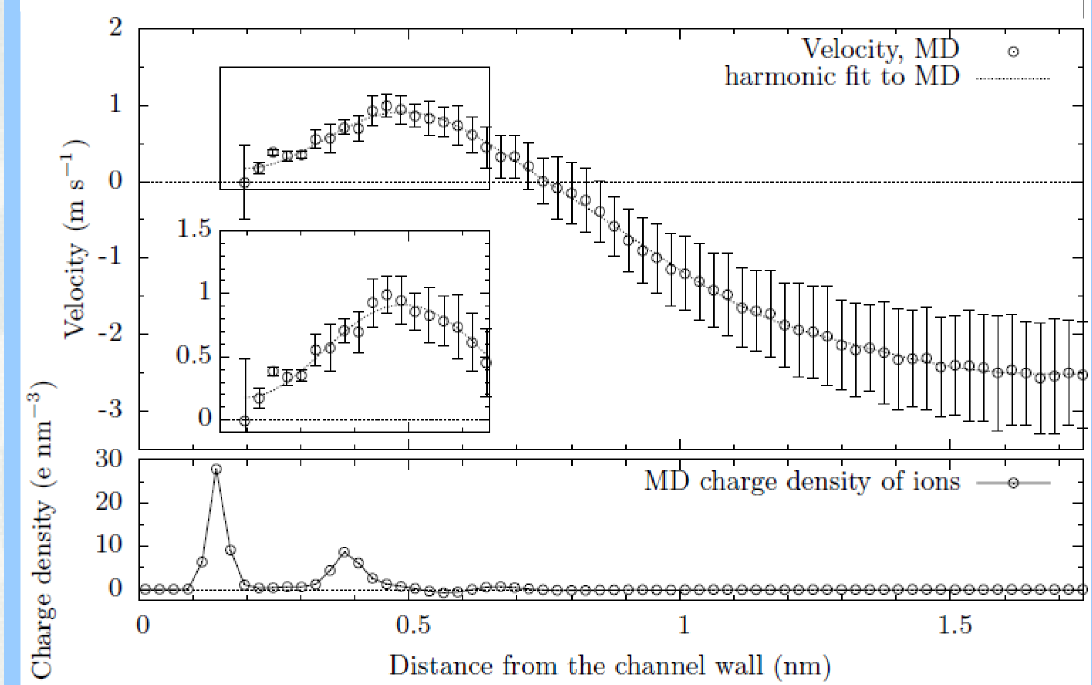


Stokes equation:

$$\frac{d}{dz}\left[\eta(z)\frac{du_x(z)}{dz}\right] = -F_d(z)$$

Dark blue line:
velocity prediction
from MD charge density,
assumes constant viscosity

Viscosity estimation



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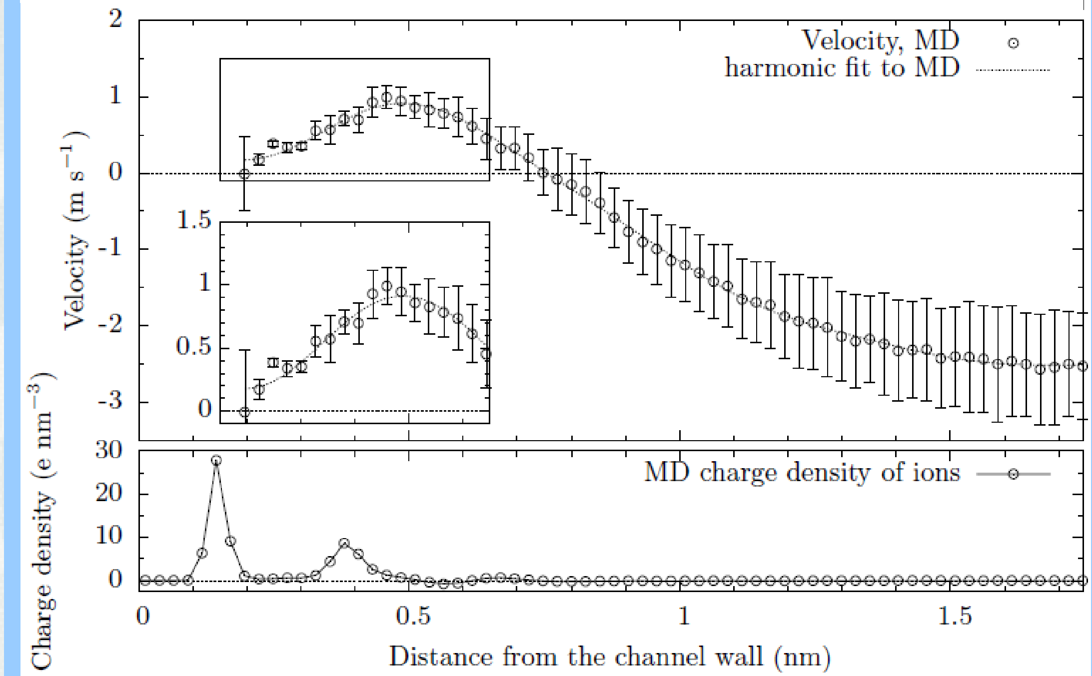

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$$\frac{d}{dz}\left[\eta(z)\frac{du_x(z)}{dz}\right] = -F_d(z)$$

Integrated:

$$\eta(z)|_{z=z_0} = \frac{-\int_0^{z_0} F_d(z)\,dz}{\left.\frac{du_x(z)}{dz}\right|_{z=z_0}}$$

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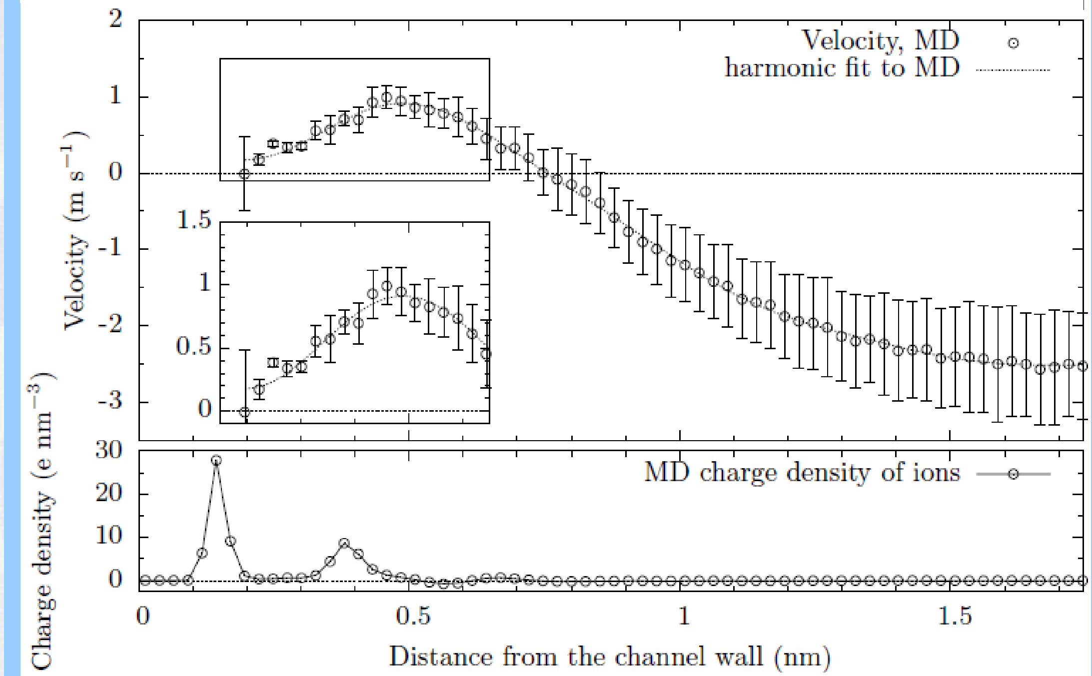

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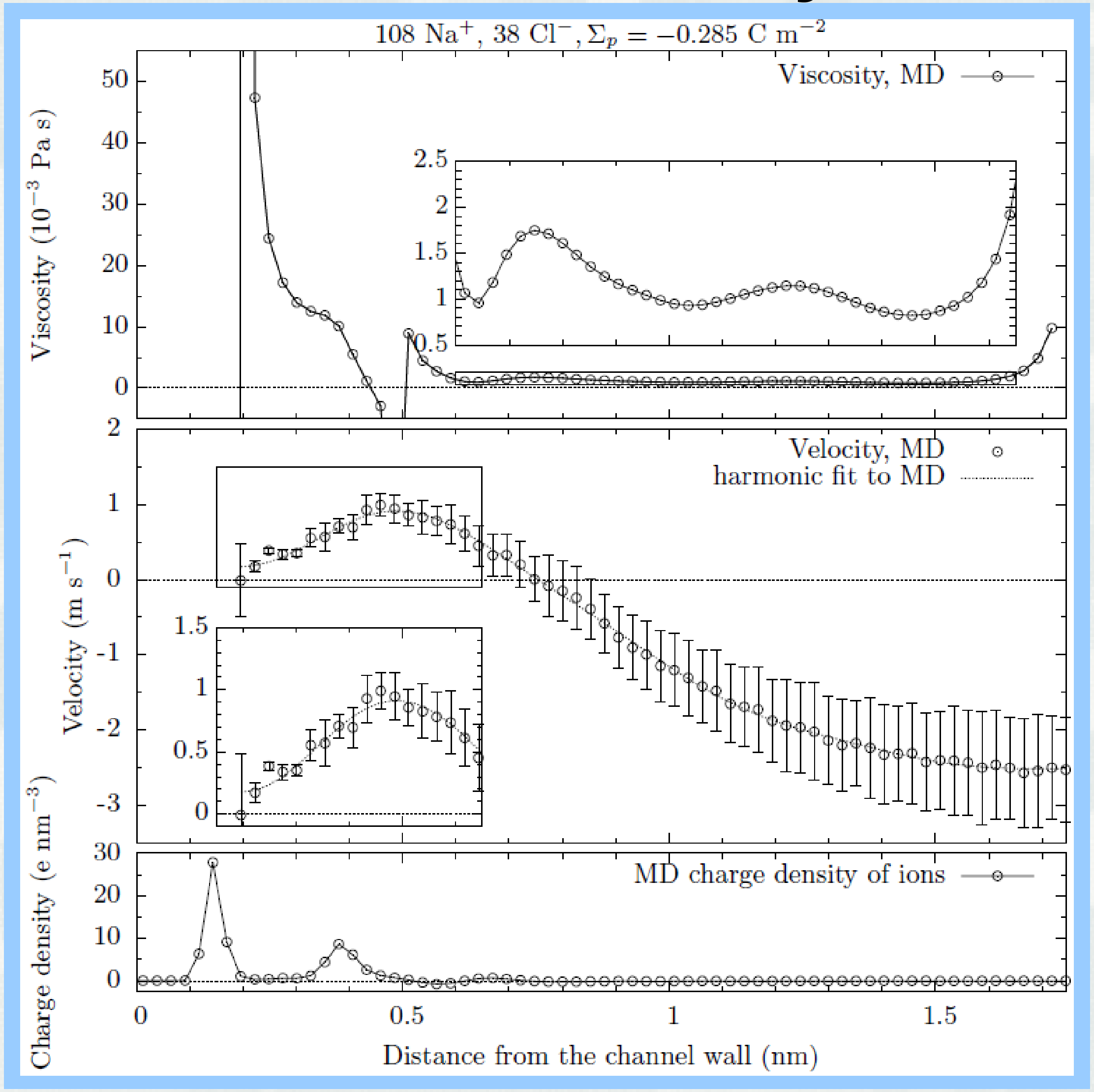
Velocity approximation:

$$u_{xfit}(z) = \sum_{n=0}^{7} a_n \cos\left(n\pi\frac{z}{h}\right)$$

J.B. Freund, J. Chem. Phys. 116(5), 2002

$$u_{\text{fit}}(y) = u_m \exp\left[\frac{(y-y_m)^4}{y_1^4}\right] + \sum_{n=0}^{11} a_n \cos\frac{\pi y n}{L}$$

Viscosity estimation



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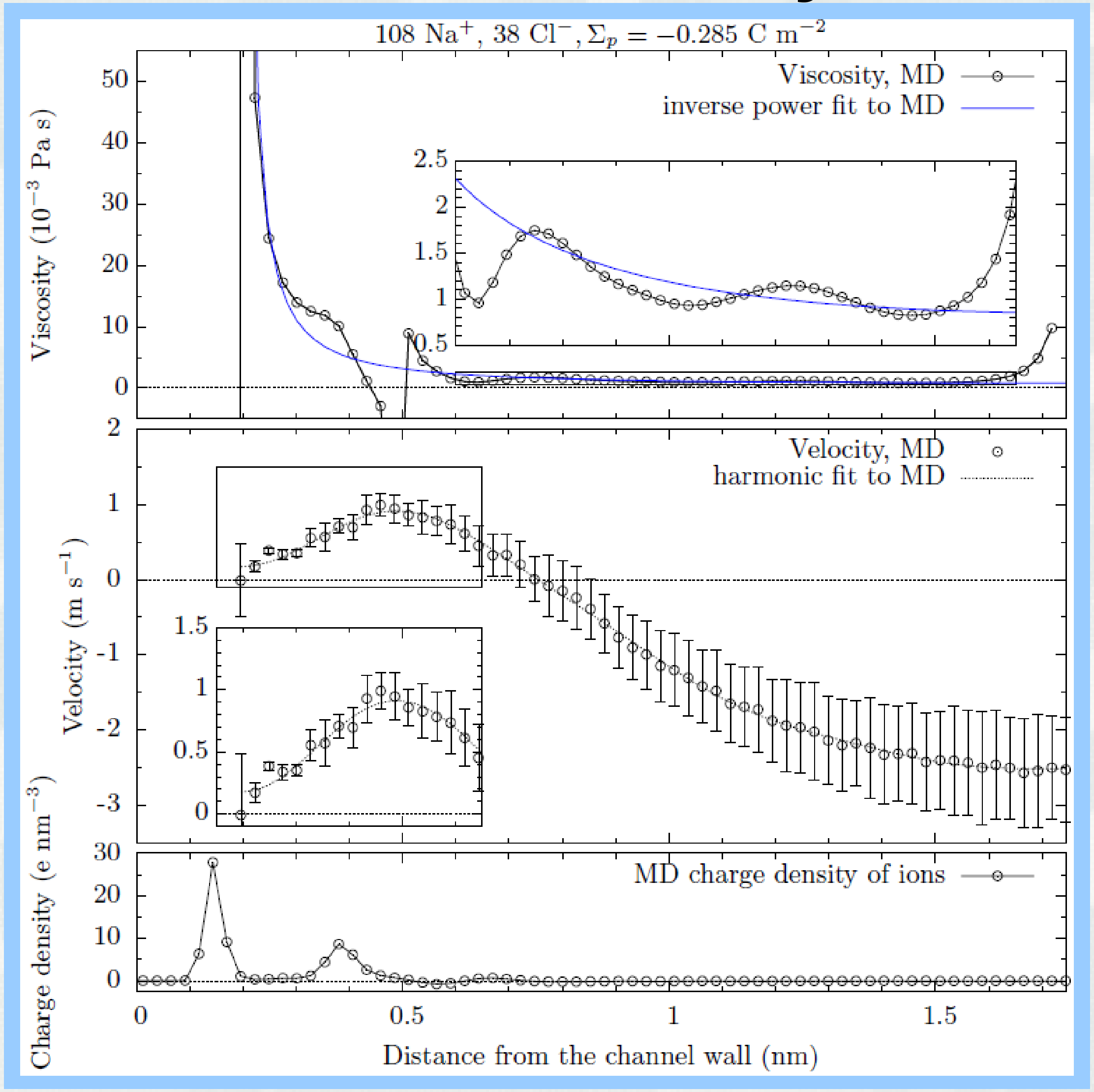

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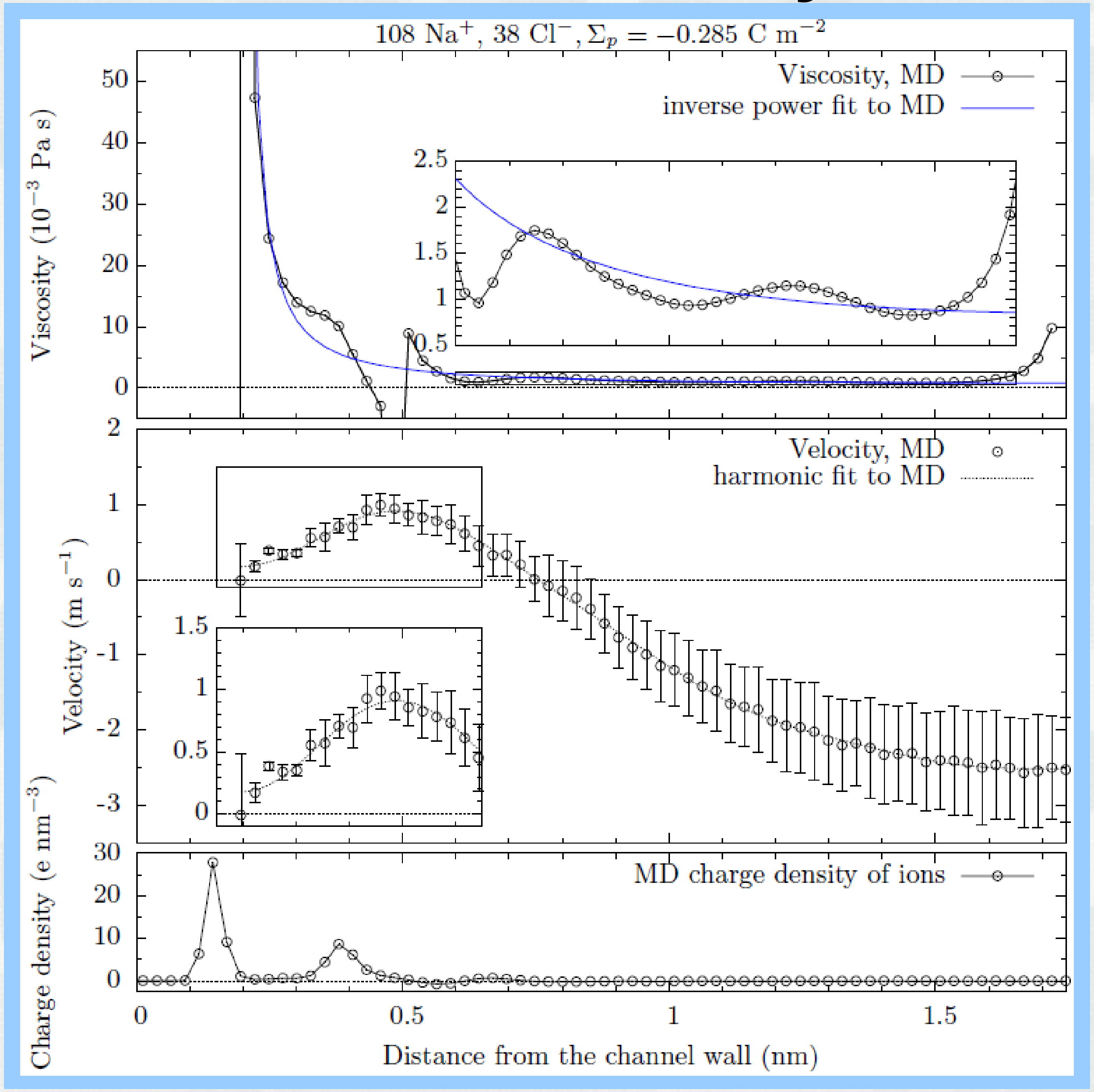

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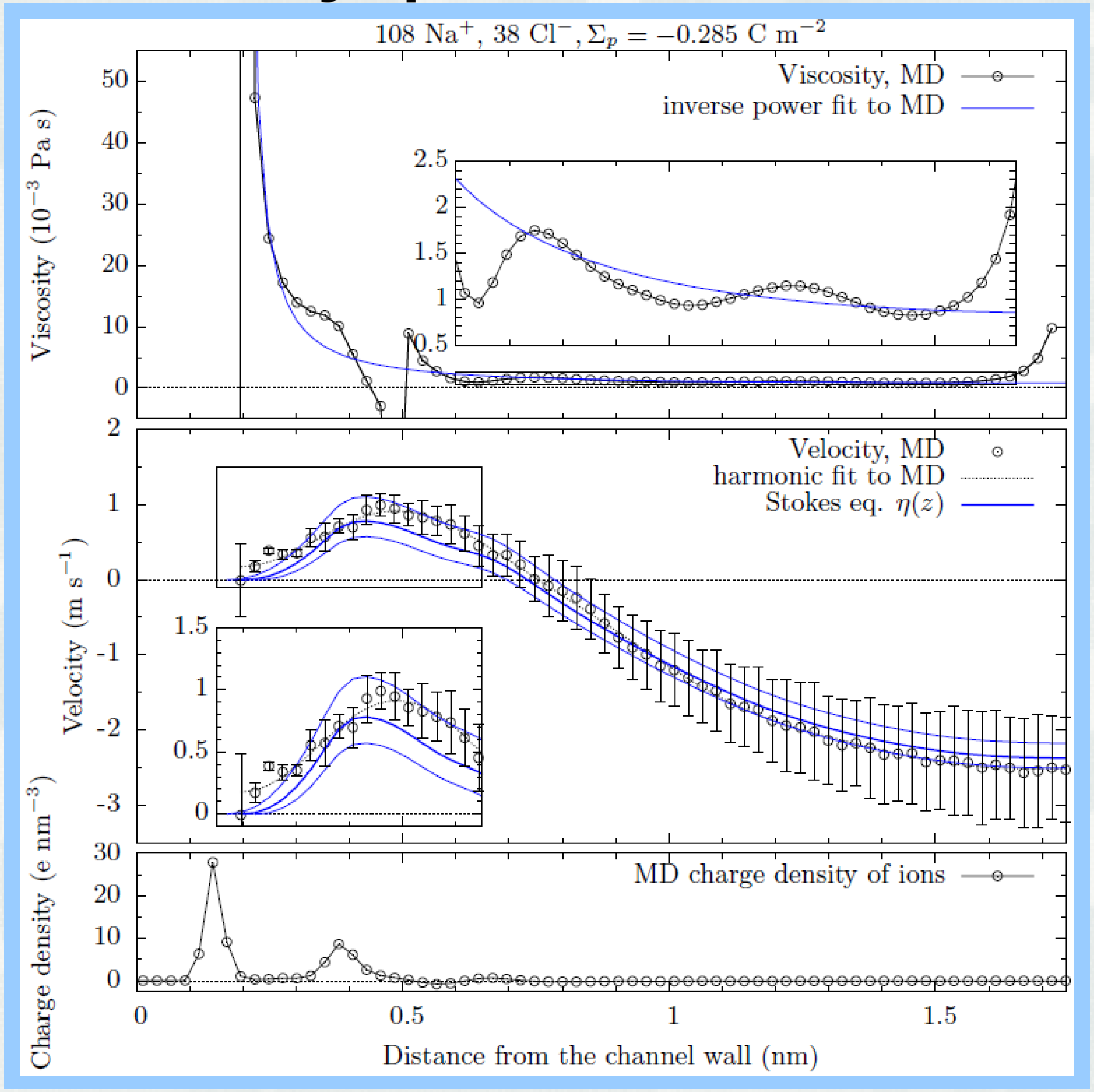
Velocity predicted from charge density



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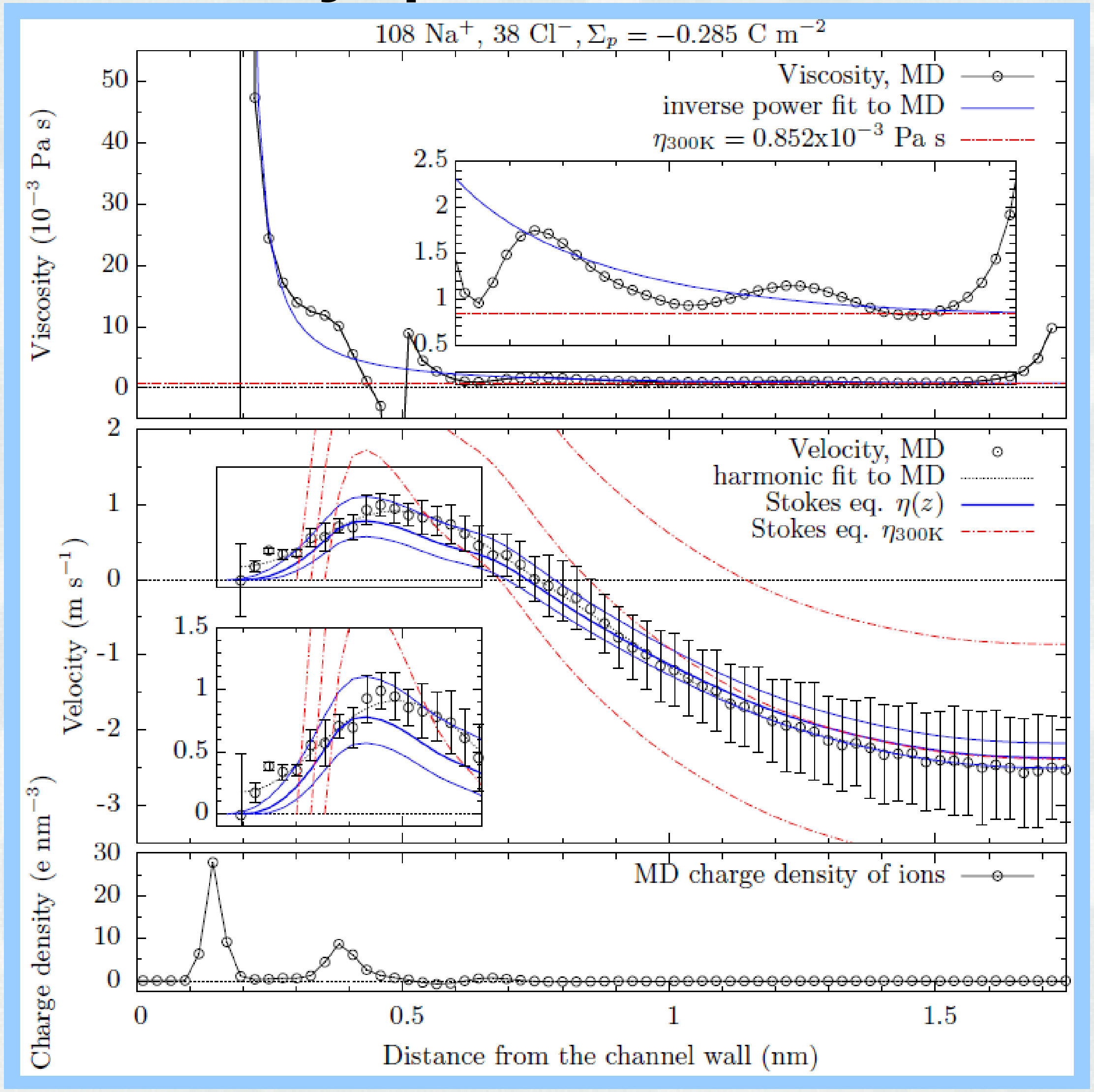

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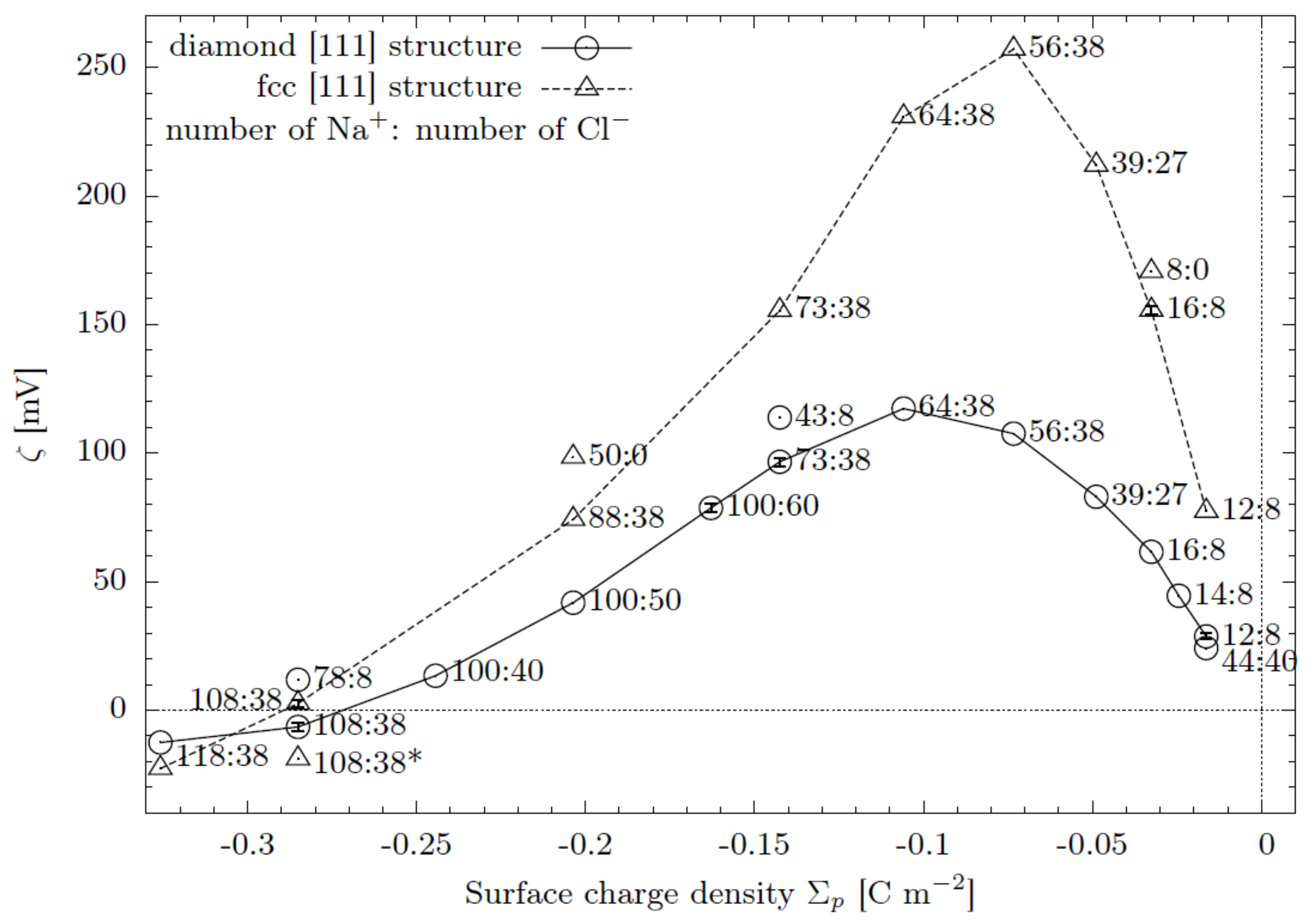
Zeta potentials vs. surf. charge density for uniform partial surface charge



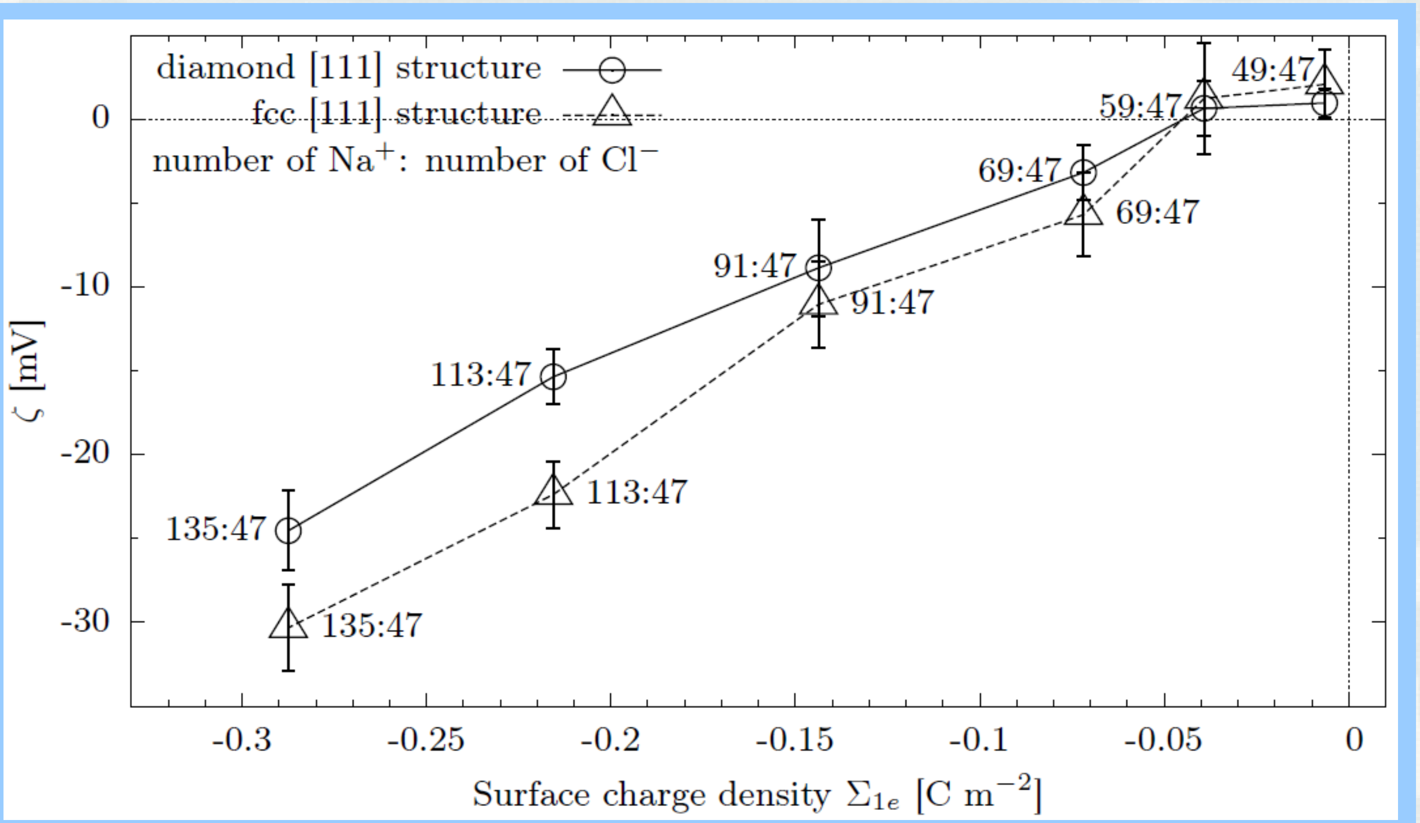
MD Zeta potential:

$$\zeta = \frac{u_x(z_{\text{center}})\eta}{\varepsilon_0 \varepsilon_r E_x}$$

Zeta potential is proportional to the water velocity in the channel center.

Assumes u_x is linear in E_x.

Zeta potentials vs. surf. charge density for discrete partial surface charge



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Conclusions

Demonstrated an improved prediction of velocity profile from charge density with non-constant viscosity estimated from MD simulations

Revealed the dependence of the flow on surface charge density, distribution, and ionic concentrations