EFFECTS OF SURFACE CHARGE DENSITY AND DISTRIBUTION ON THE NANOCHANNEL ELECTRO-OSMOTIC FLOW

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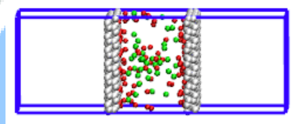
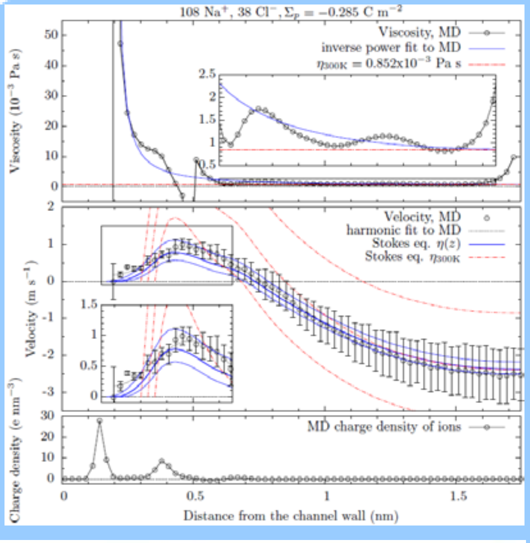
Senior Research Scientists

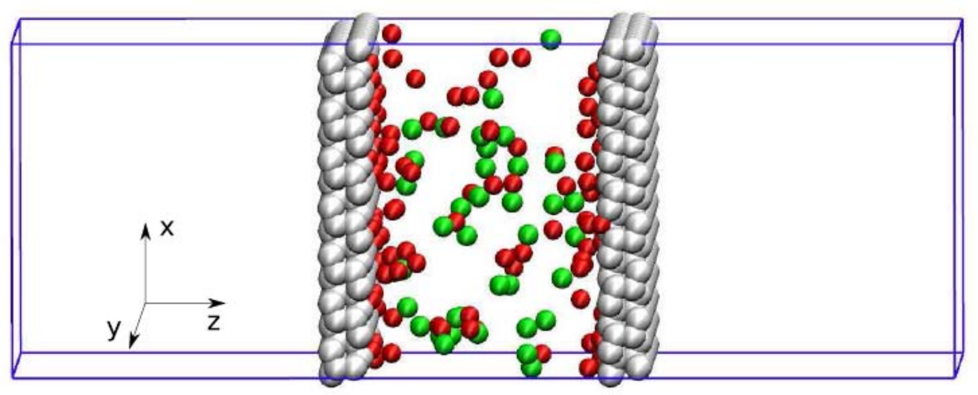
GSL, U.S. Army ERDC Vicksburg, MS



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

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





US Army Corps of Engineers

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CAVS

Other project

Development of MEAM potential for Al-Si-Mg-Cu-Fe alloys

B. Jelinek, S. Groh, A. Moitra, M. Horstemeyer, J. Houze, S-G. Kim, G. Wagner, M. Baskes

http://arxiv.org/abs/1107.0544

Scripts to reproduce some of the potential tests

http://code.google.com/p/ase-atomistic-potential-tests

using Atomistic Simulation Environment (ASE)

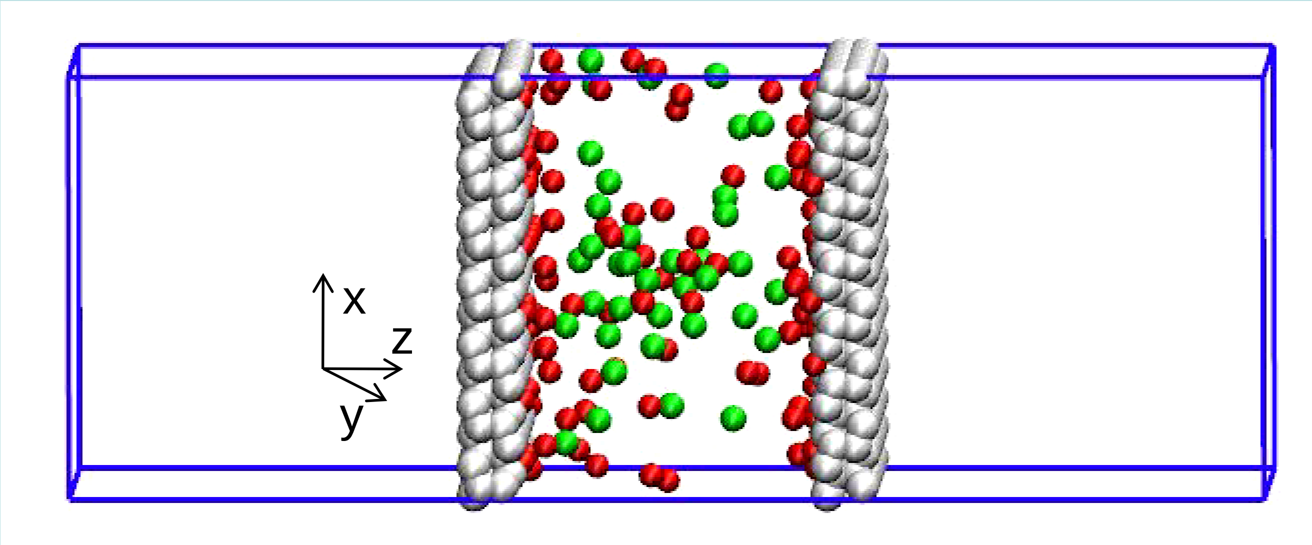
https://wiki.fysik.dtu.dk/ase

motivation for using ASE - talk at the NIST 2011 workshop

http://www.ctcms.nist.gov/potentials/activities.html

CAVS cyberinfrastructure site https://ccg.hpc.msstate.edu

Electro-osmotic flow model



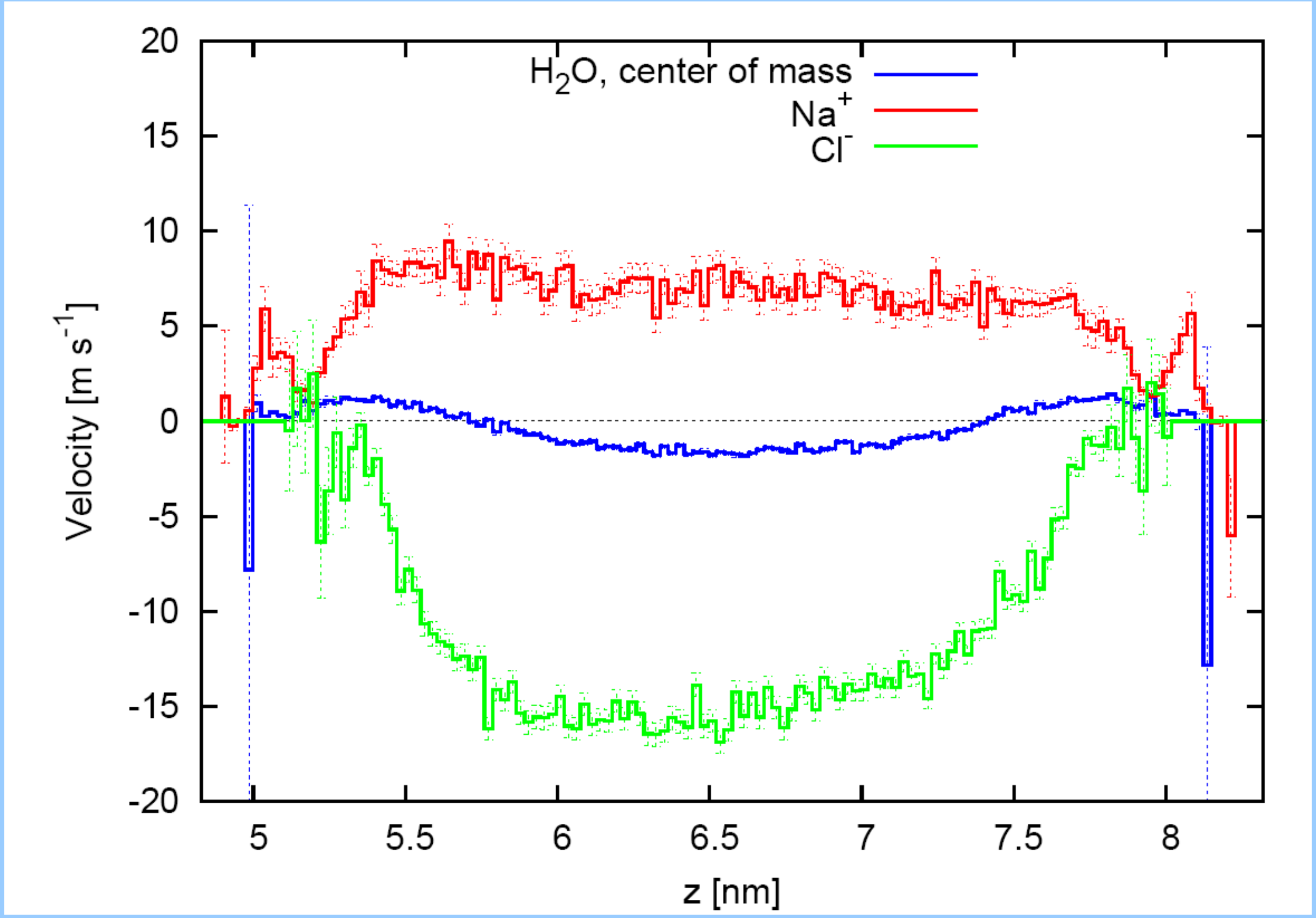
Fixed Si channel walls, innermost layer charged negatively

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

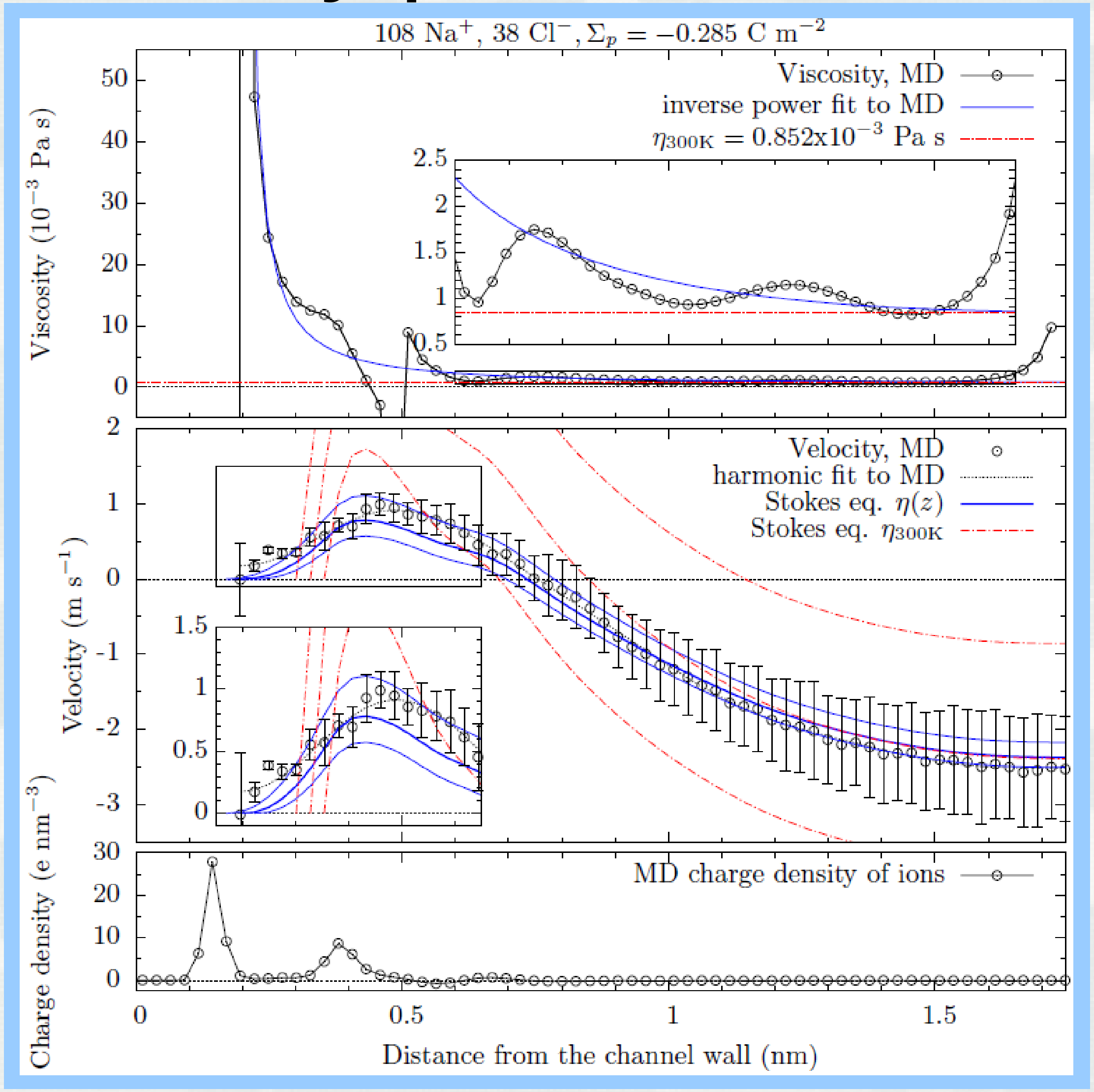
108 Na^+, 38 Cl^-, 2144 SPC/E H_2O molecules (not shown)

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:

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

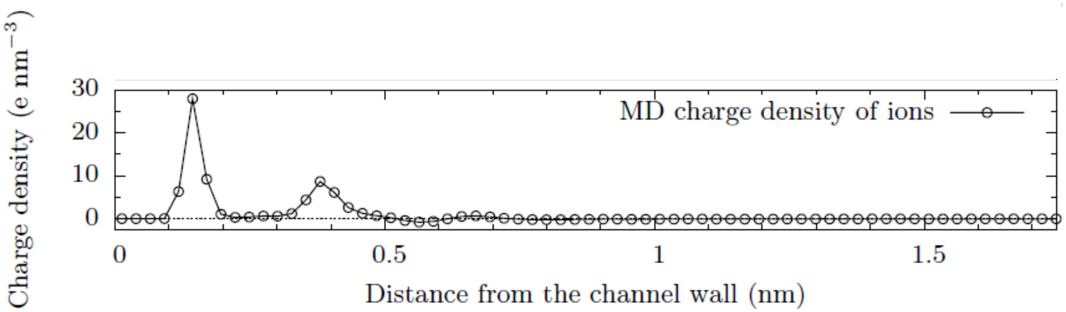
Blue:
inverse power viscosity

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

Red:
constant viscosity

Black circles:
Molecular Dynamics

Velocity predicted from charge density



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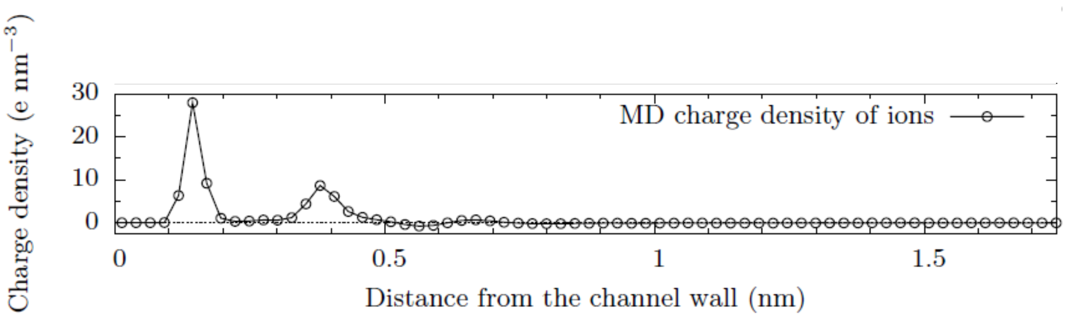

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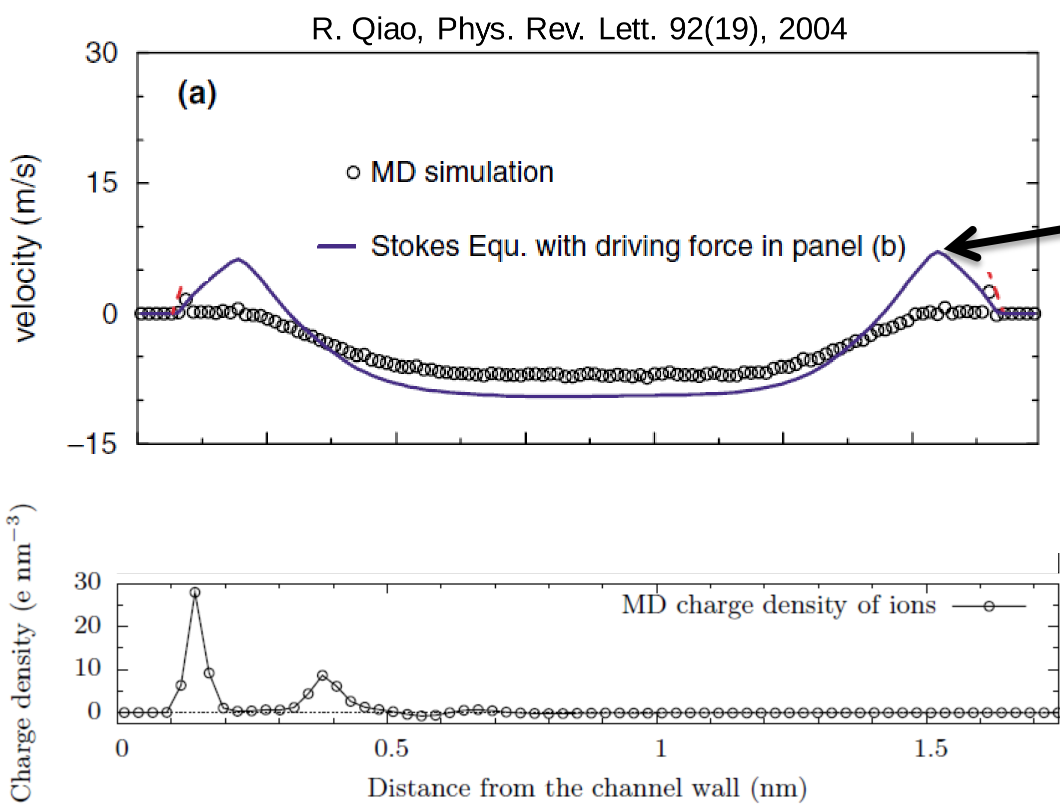

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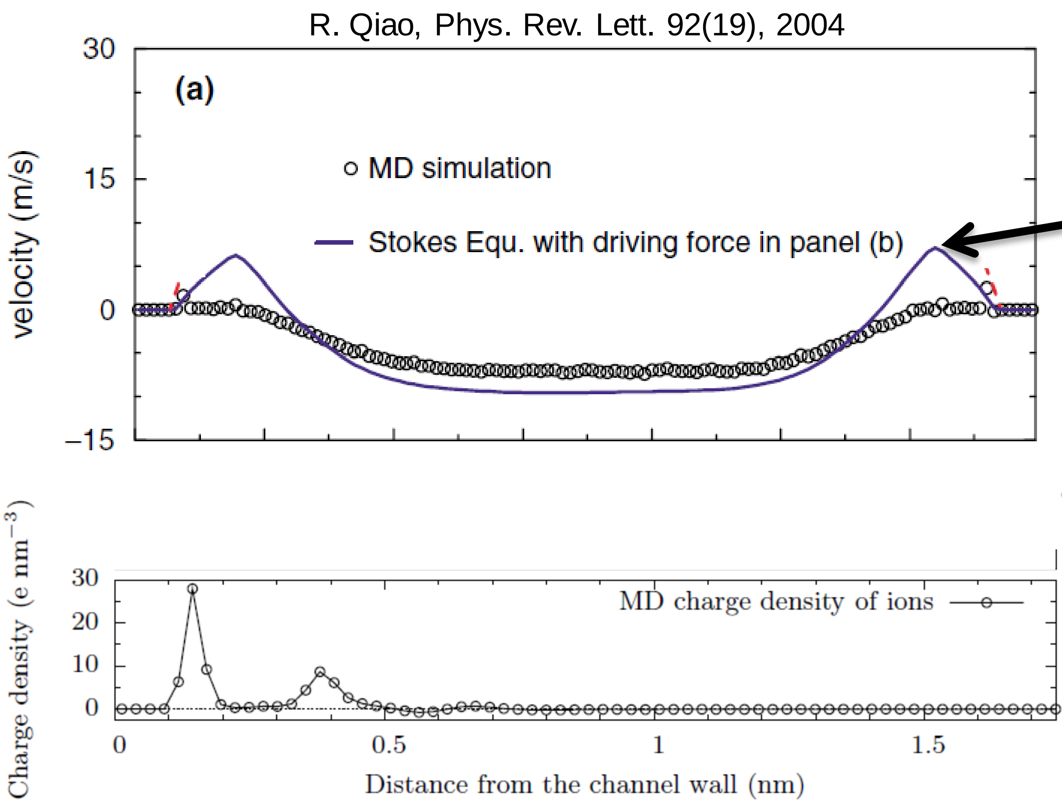
Dark blue line:
velocity prediction
from MD charge density

Velocity predicted from charge density

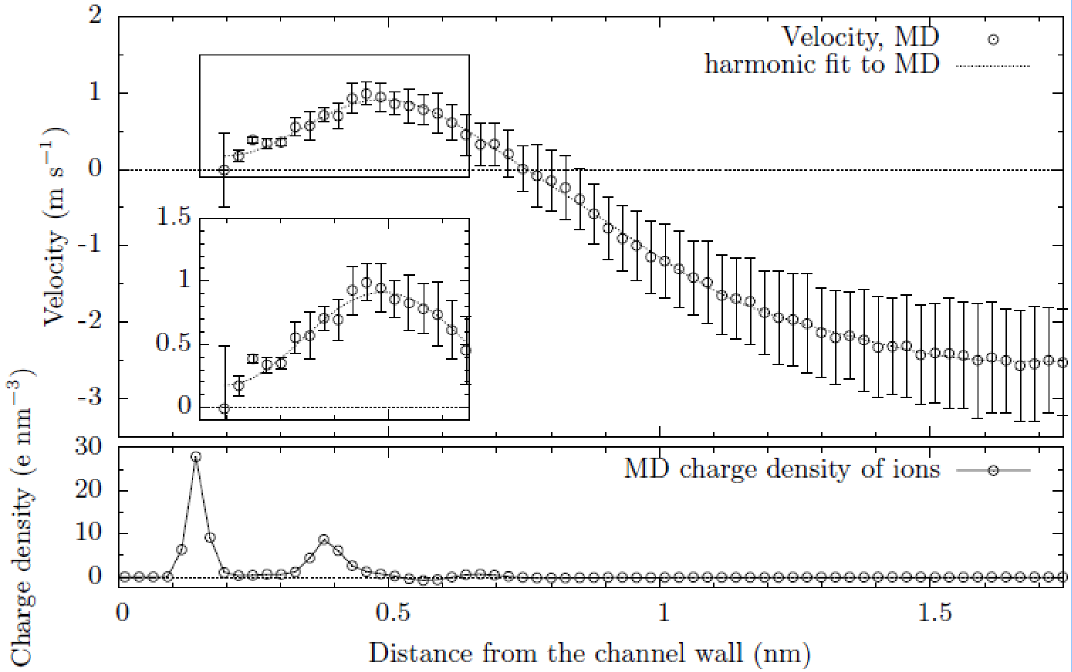


Stokes equation:

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

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

Viscosity estimation



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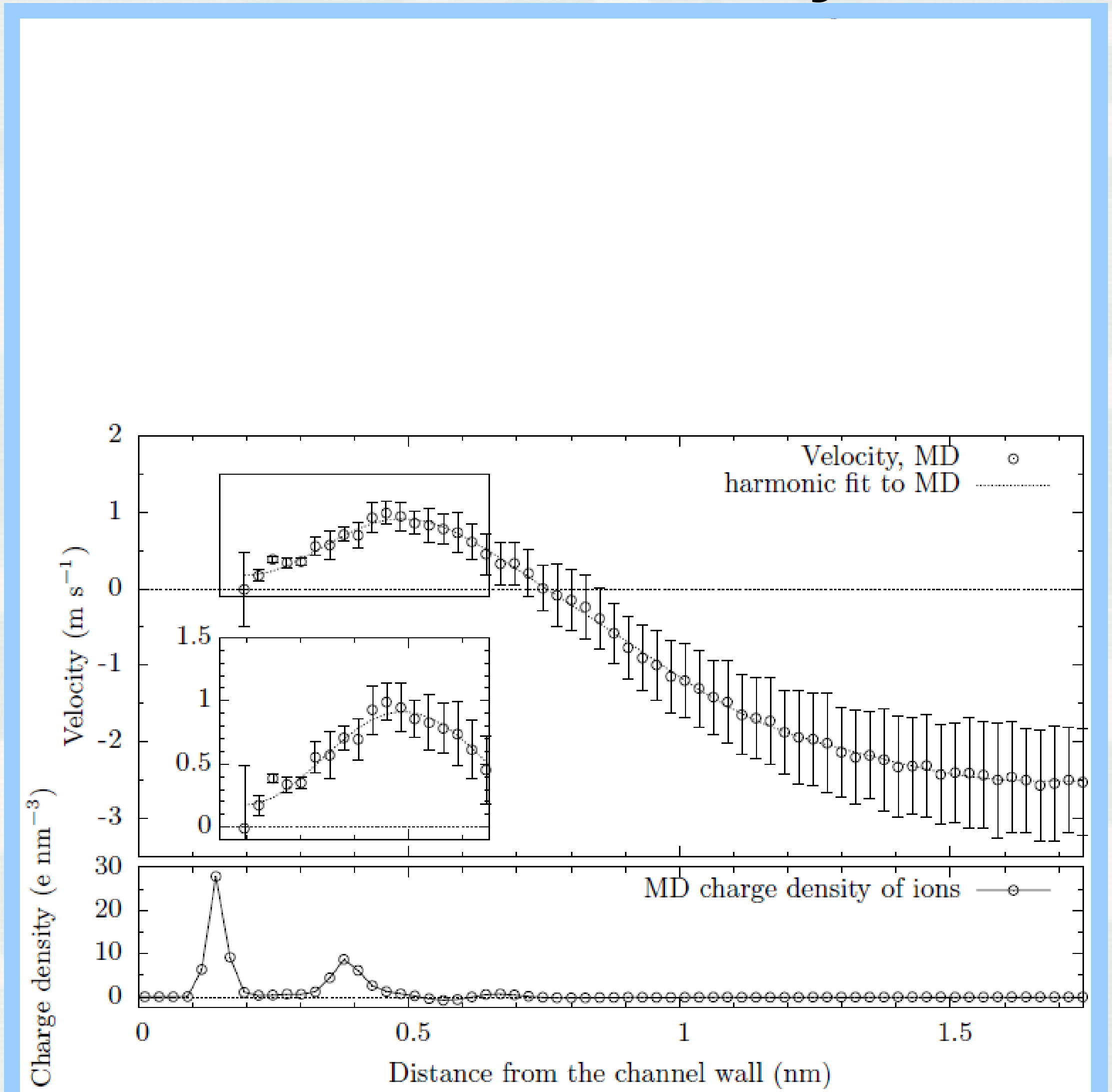

Stokes equation:

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

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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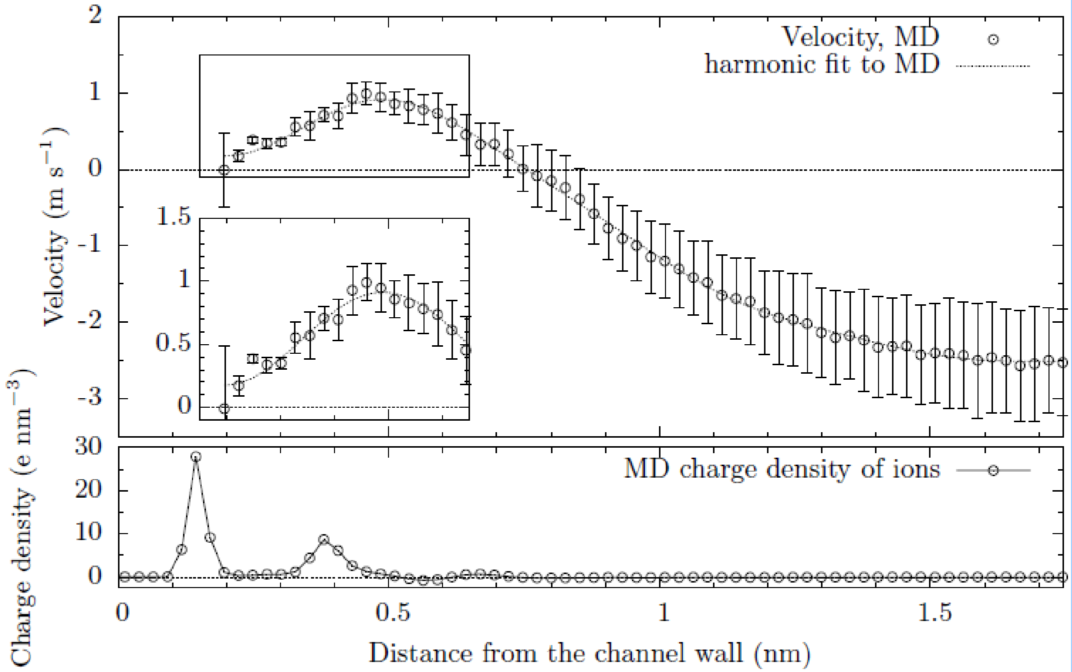

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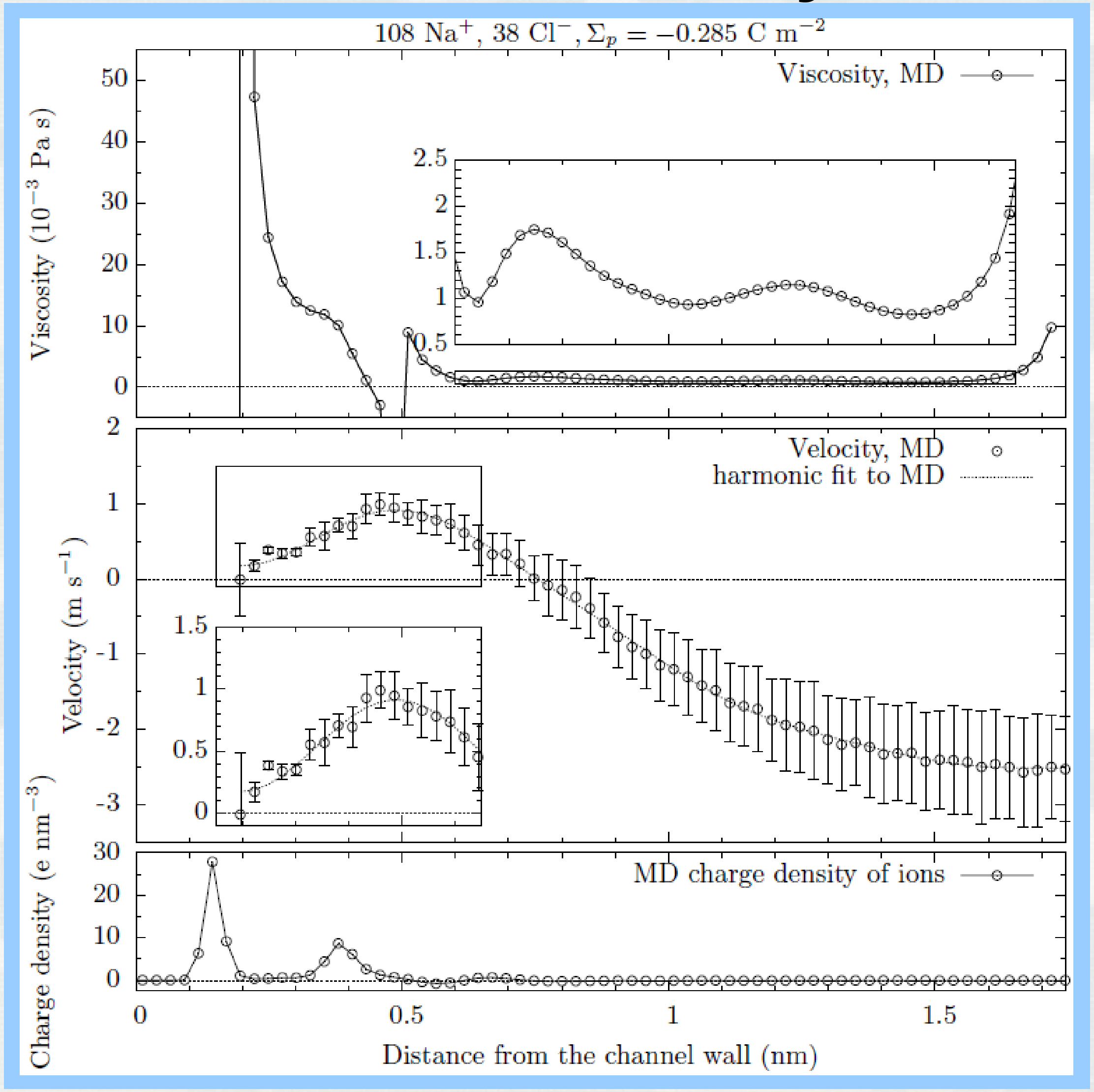
Velocity approximation:

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

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

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

Viscosity estimation



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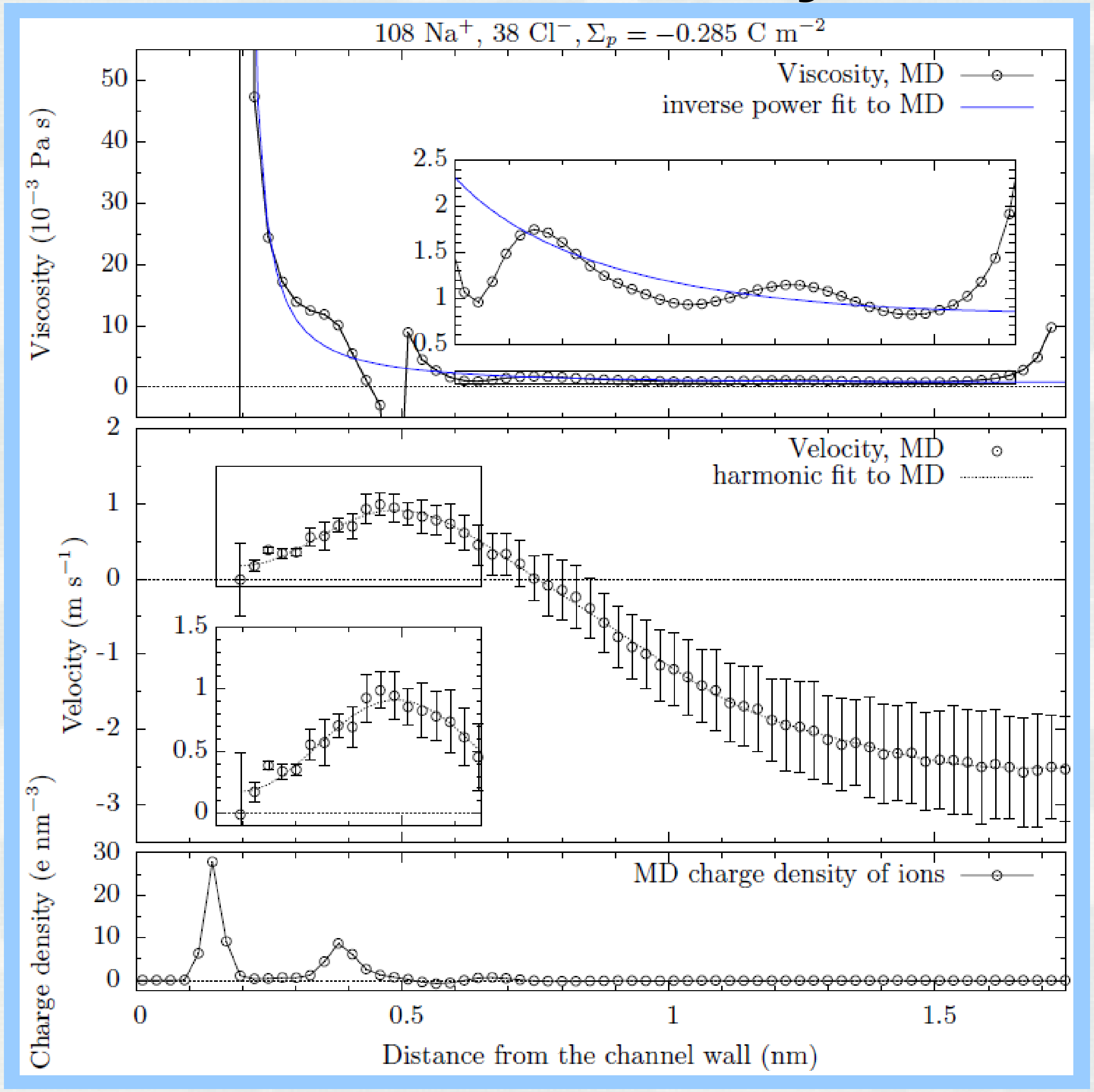

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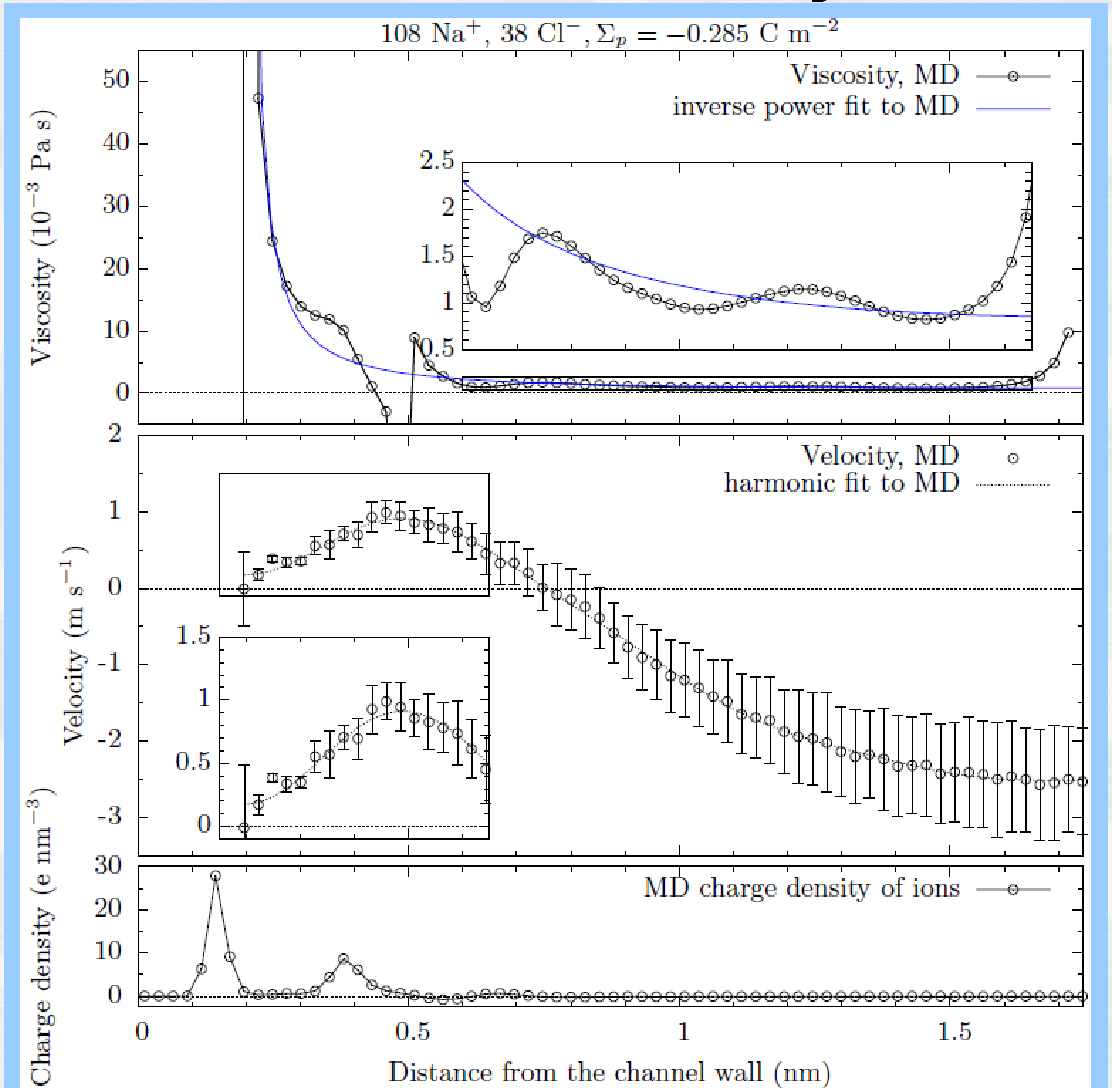

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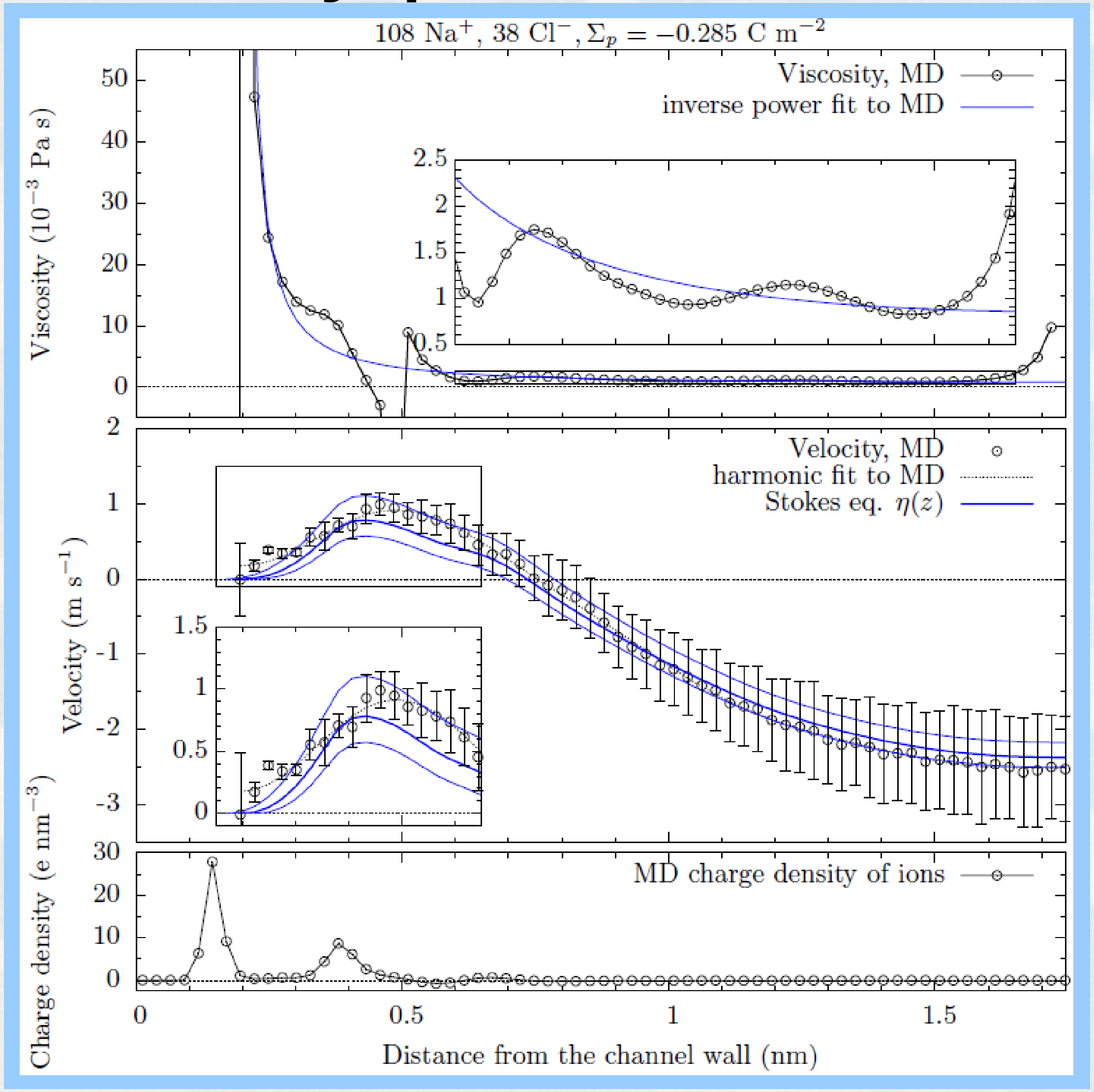
Velocity predicted from charge density



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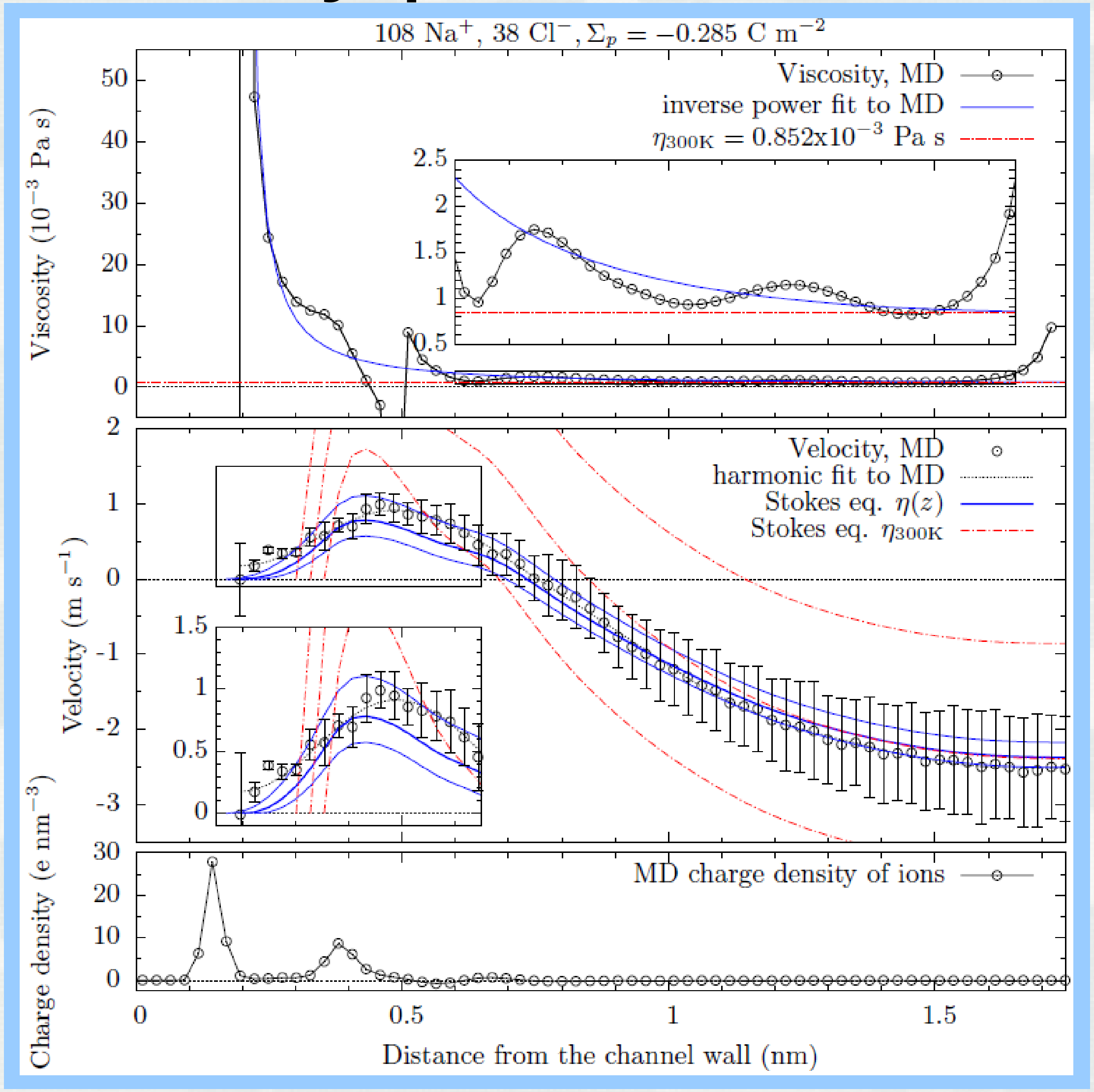

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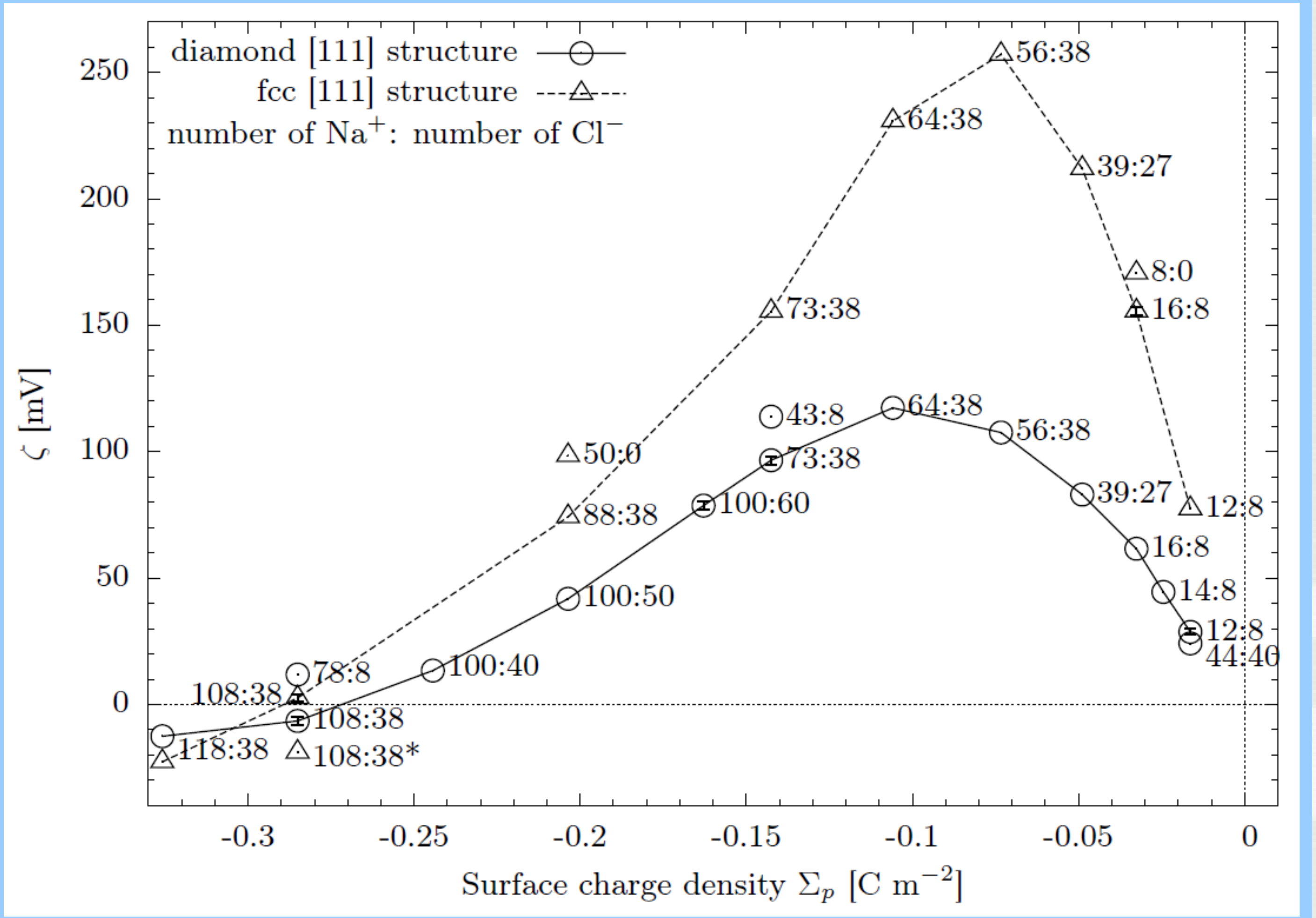
Zeta potentials vs. surf. charge density for uniform partial surface charge



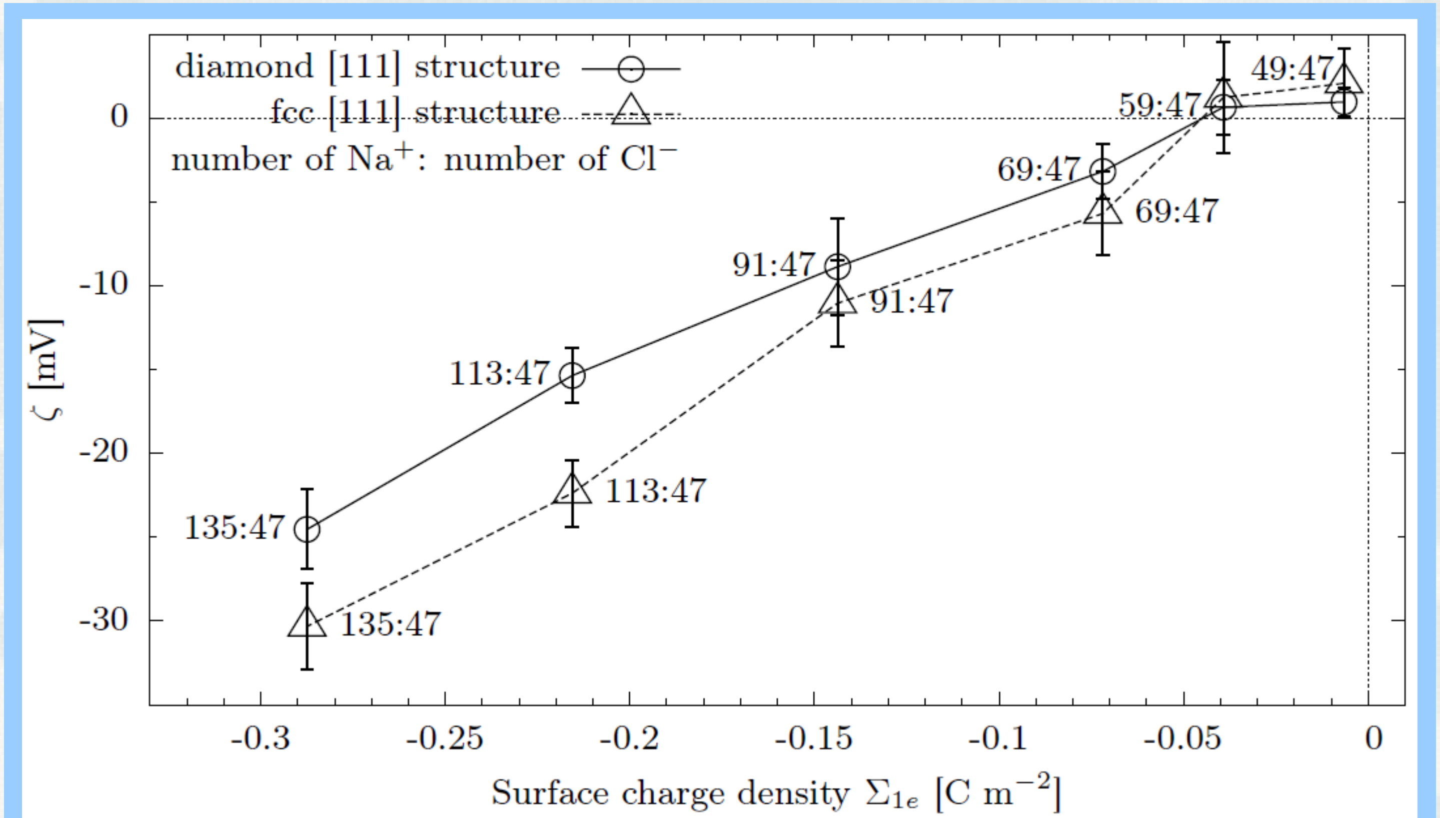
MD Zeta potential:

$$\zeta = \frac{u_x(z_{\mathrm{center}})\eta}{\varepsilon_0\varepsilon_{\mathrm{r}}\mathrm{E}_x}$$

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

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Conclusions

Studied factors significantly affecting nanochannel electro-osmotic flow by MD simulations

Obtained velocity profiles, ionic concentrations, and viscosity profiles

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

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