

ABSTRACT

Title of thesis: ENERGY CONVERSION
IN NANOCHANNELS GRAFTED
WITH POLYELECTROLYTE AND
POLYZWITTERION BRUSHES

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A continuous mission in the sciences is the never-ending search for more energy and fuel. As time brings the reality of how limited natural resources are, we seek to expand to more synthetic methods of preserving and converting energy. Prevalent applications of renewable energy include solar energy, wind power, tidal power, and hydropower to list a few. It is no surprise that several of these applications stem from the involvement of fluid flow and the fluid pressure. This thesis explores a specific method of energy conversion in charged nanochannel flows of electrolytic solution, a subject that has gained great attention in recent years.

This particular method of nanofluidic energy conversion inside a charged nanochannel is an example of *Electrokinetic Energy generation* in pressure-driven liquid trans-

port. A charged nanochannel in contact with an electrolyte solution develops an *Electric Double Layer (EDL)* of charge where the number of counterions (ions of charge opposite in sign to that of the nanochannel wall) is much larger than the number of coions (ions of charge identical in sign to that of the nanochannel wall) in order to screen the wall charge. In presence of a pressure-driven flow, the ions within the EDL are advected downstream. The counterions number density being much larger than the coions, such a downstream migration would imply the accumulation of a net charge in the downstream direction, thereby triggering an axial electric field. This electric field when multiplied with the current generated due to the streaming of the ions would lead to an energy generation – this energy generation is effectively an example of *Electrochemomechanical Energy conversion*, where the mechanical energy of the pressure-driven flow and the chemical energy of the EDL gets converted into an electrical energy.

The purpose of this thesis is to explore the such *Electrokinetic Energy Conversion* in nanochannels grafted with pH-responsive charged polyelectrolyte (PE) brushes.

Grafting of nanochannels with polyelectrolyte (PE) brushes, invariably attribute a “smartness” to the nanochannels that have been used for a plethora of applications ranging for ion and biosensing, gating of ion transport, current rectification, fabrication of nanofluidic diodes and nano-actuators, etc. All these applications strictly depend on the modification of the *ionic current* by the presence of the PE brushes. On the contrary, the energy generation/conversion that we study here is a rare example where we utilize the *Electrohydrodynamic (EHD)* transport in brush-functionalized

nanochannels.

In this thesis, we experiment with parameters that would provide significant electrochemomechanical energy conversion in the presence of a pressure-driven background transport. We've gathered the optimal parameters to result in a 4-5% energy conversion efficiency. This is possible when the PE brushes exhibit a pH-dependent charge density.

Further, we extend our research by determining the possible electrochemomechanical energy conversion in a nanochannel grafted with polyzwitterionic (PZI) brushes. PZI brushes are capable of inducing a significantly high charge on both acidic and basic solutions. This allows electrokinetic induced power to be accessible over a wide range of pH values, as opposed to being confined to a narrow pH range compared to other EDL channels.

This thesis therefore sheds light on the smartness of nanochannels and their capabilities to generate power. We anticipate that our results will be able to provide a way for energy to be induced and produced in nanochannel-related applications, and maybe even find means to be a measure for developing more sustainable energy in larger scale applications.