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The Dependence of Diffusio-Phoretic Mobility and Aggregation Properties of Proteins on Intermolecular Interaction in Confined System

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Abstract: Phoretic flow can be generated by different types of gradient (e.g. temperature, concentration, or charge gradient) [1-3]. Within micro-to-nano confined system, the diffusio-phoretic property for proteins differs dramatically from that obtained in bulk condition, due to concentration fluctuation that emerges at microscopic level induced by specific and nonspecific interactions between protein and co-solute [4-5]. The phoretic mobility of protein individuals and complex in solute gradients can be theoretically described by continuum model [1-2] that neglects microscopic heterogeneity and determined experimentally by microfluidics [6], but the underlying mechanism of diffusio-phoretic motion for confined protein still remains unclear.

Our approach to this challenge is to combine real-time, label-free observations on microfluidic devices [7] and molecular dynamics simulations [8-9] driven by implicitly imposed forces, to analyze the time evolution of dynamics and distribution for proteins in solute gradients and determine the controlling parameters for diffusio-phoretic mobility. We also design a simple model of spherical colloid submerged and fixed in out-of-equilibrium fluid consisting of solute and solvent, to characterize the sensitive dependence of the rate of diffusio-phoretic flow created by the colloid on solute concentration and interaction strength at microscopic level. We present general features for the fluctuations of number and force density of fluid around the colloid. Suitable values of controlling parameters that maximize the diffusio-phoretic mobility are determined, which cannot be properly measured by traditional continuum approximations. The results explain the microscopic mechanism of diffusio-phoretic motion for proteins in confined system and the following focusing or aggregation that may lead to degenerative diseases like Alzheimer. It also helps to develop low-cost, high-precision microfluidic chips for protein separation and purification.

Keywords: Diffusio-phoresis; dynamics and regulation; label-free microfluidics; molecular simulation

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References

1. Anderson JL, Lowell ME, Prieve DC. Motion of a particle generated by chemical gradients Part 1. Non-electrolytes. *Journal of Fluid Mechanics* **1982**, 117: 107-121.
2. Khair AS. Diffusiophoresis of colloidal particles in neutral solute gradients at finite Péclet number. *Journal of Fluid Mechanics* **2013**, 731: 64-94.
3. Stout RF, Khair AS. Influence of ion sterics on diffusiophoresis and electrophoresis in concentrated electrolytes. *Physical Review Fluids* **2017**, 2(1): 014201.
4. Ault JT, Warren PB, Shin S, Stone HA. Diffusiophoresis in one-dimensional solute gradients. *Soft Matter* **2017**, 13(47): 9015-9023.
5. Eijkel JC, van den Berg A. Nanofluidics and the chemical potential applied to solvent and solute transport. *Chemical Society Reviews* **2010**, 39(3): 957-973.
6. Arosio P, Müller T, Rajah L, Yates EV, Aprile FA et al. Microfluidic diffusion analysis of the sizes and interactions of proteins under native solution conditions. *ACS nano* **2015**, 10(1): 333-341.
7. Challa PK, Peter Q, Wright MA, Zhang Y, Saar K et al. Real-time intrinsic fluorescence visualization and sizing of proteins and protein complexes in microfluidic devices. *Analytical chemistry* **2018**, 90(6): 3849-3855.
8. Liu Y, Ganti R, Frenkel D. Pressure gradients fail to predict diffusio-osmosis. *Journal of Physics: Condensed*

Matter **2018**, 30(20): 205002.

9. Yoshida H, Marbach S, Bocquet L. Osmotic and diffusio-osmotic flow generation at high solute concentration. II. Molecular dynamics simulations. *The Journal of chemical physics* **2017**, 146(19): 194702.