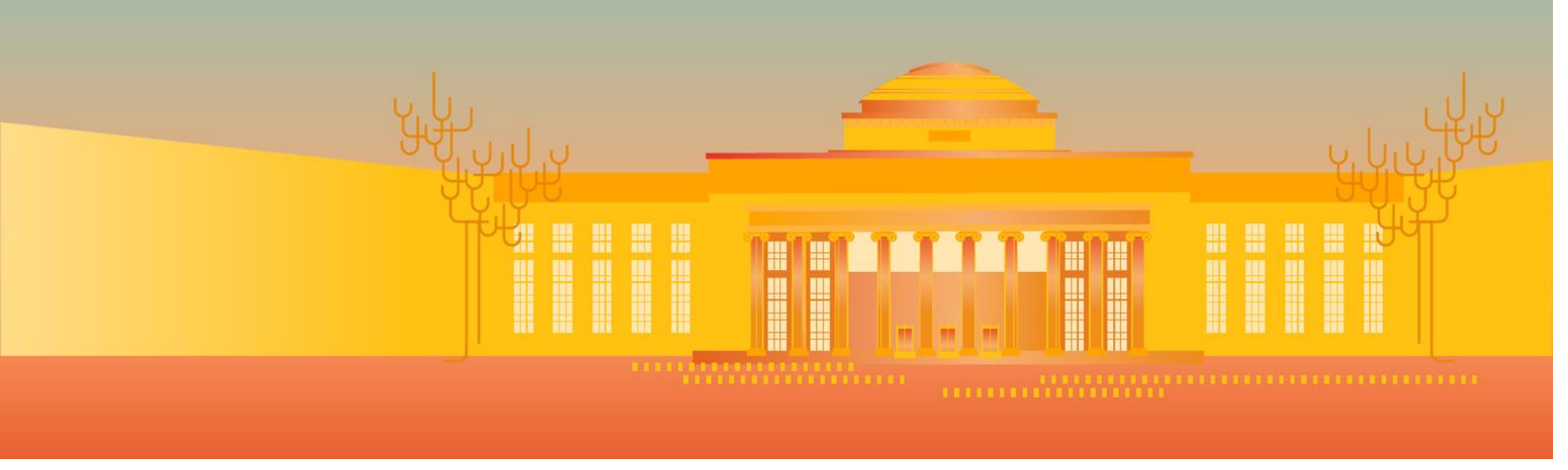

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PHOTOCATALYTIC SELF-PROPELLED MICROMOTORS FOR ACCELERATION OF ADVANCED OXIDATION PROCESSES

Yangyuan Ji[1], Matthew Tao[1,2], Yuhang Fang[1], Harshita Masand[3], David Warsinger[1], Jeffrey Moran[4]

[1]School of Mechanical Engineering & Birck Nanotechnology Center, Purdue University; [2]Department of Physics, University of California, Berkeley

[3]Department of ME&MS, Indian Institute of Technology Bombay; [4]Department of Mechanical Engineering, George Mason University

BACKGROUND

- Energy-efficient water treatment is crucial to effectively addressing climate change
- Advanced Oxidation Processes (AOPs) are a versatile class of water treatment methods that can eliminate Contaminants of Emerging Concern (CECs), which survive traditional water treatment methods (e.g. reverse osmosis)
- A common AOP employs UV light and photocatalytic TiO_2 nanoparticles to produce hydroxyl radicals (·OH) to degrade pollutants
- AOP ADVANTAGES: (1) *mineralize* contaminants (permanently eliminating the threat they pose), leaving no toxic sludge behind. (2) applicable to wide range of pollutants (**including CECs**) because of non-specificity of ·OH radicals
- AOP CHALLENGES: (1) mass transfer limitations, (2) short lifetime of ·OH radicals, (3) recovery of photocatalysts from treated water
- Here, we test the hypothesis that **the degradation of pollutants is accelerated if 400-nm TiO_2 particles *propel themselves* through the water using UV light (already present in TiO_2 AOPs) as fuel, vs. non-propelled particles.**

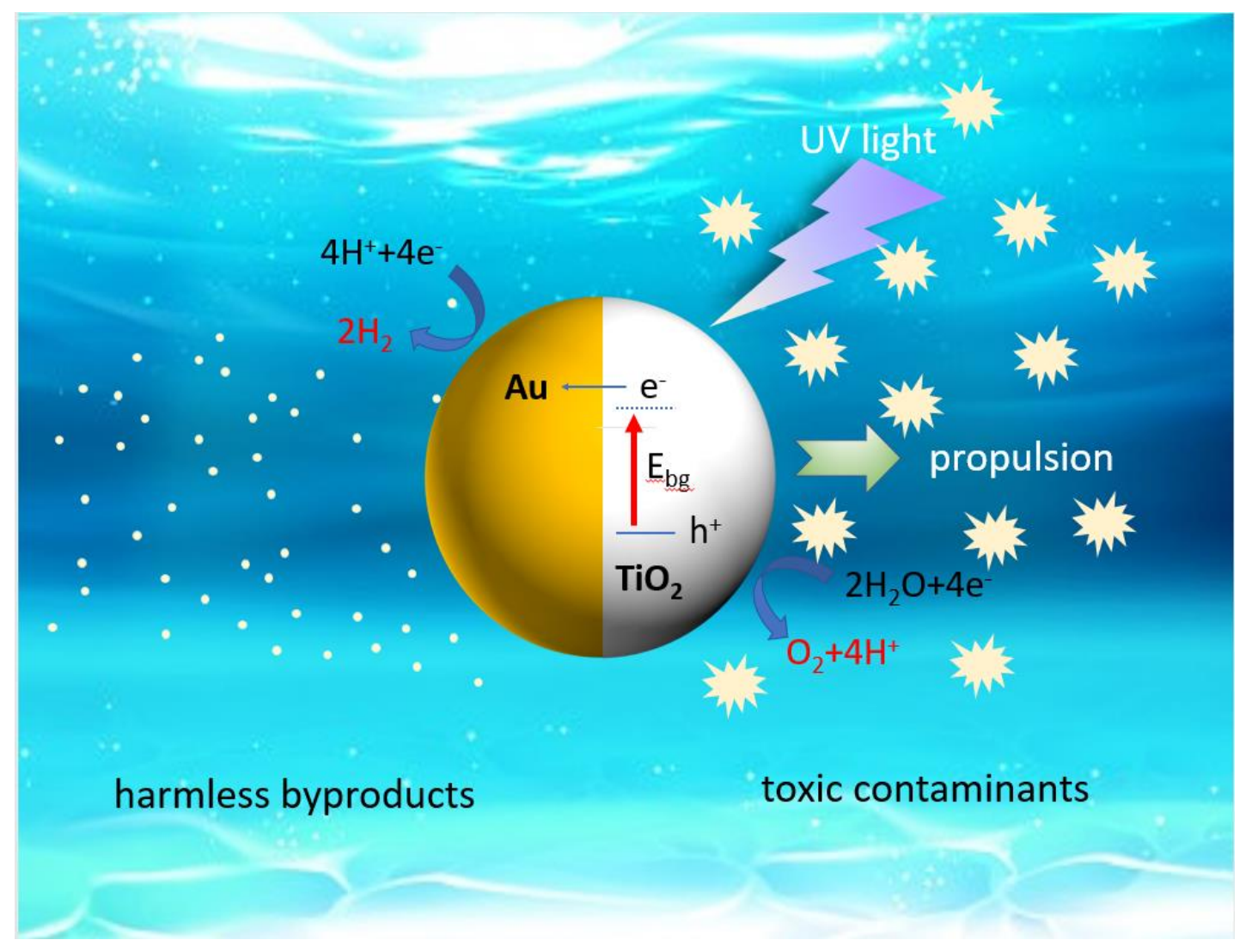
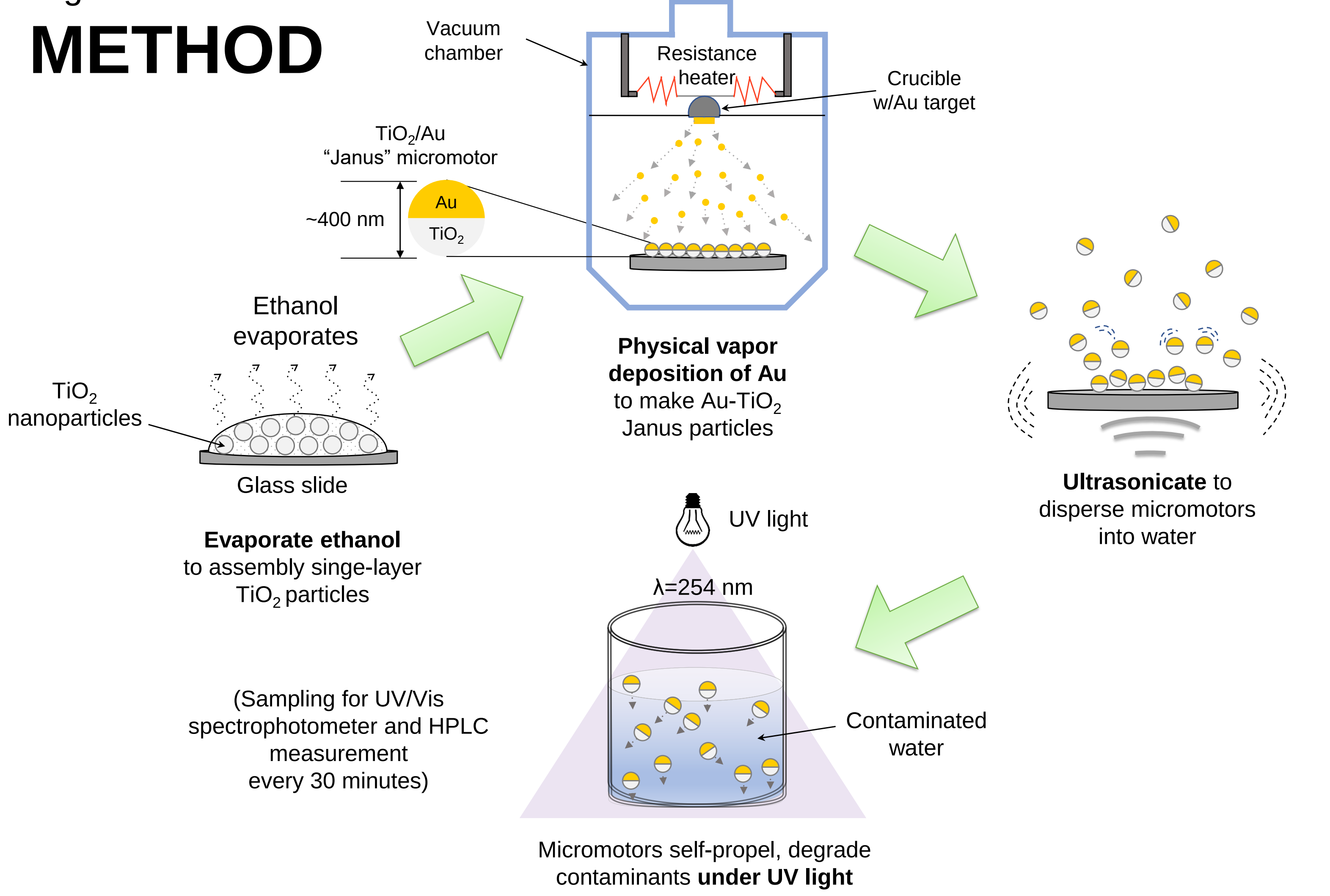


Figure 1: Schematic of titanium dioxide/gold (TiO_2/Au) micromotor, first demonstrated by Dong et al. [1]. Using incoming UV light as a fuel, the micromotor propels itself in water, degrading contaminants into harmless byproducts. As shown, motion is from left to right.

METHOD



Evaporate ethanol to assembly singe-layer TiO_2 particles

Physical vapor deposition of Au to make Au-TiO_2 Janus particles

Ultrasonicate to disperse micromotors into water

Micromotors self-propel, degrade contaminants **under UV light**

(Sampling for UV/Vis spectrophotometer and HPLC measurement every 30 minutes)

POLLUTANT DEGRADATION RESULTS

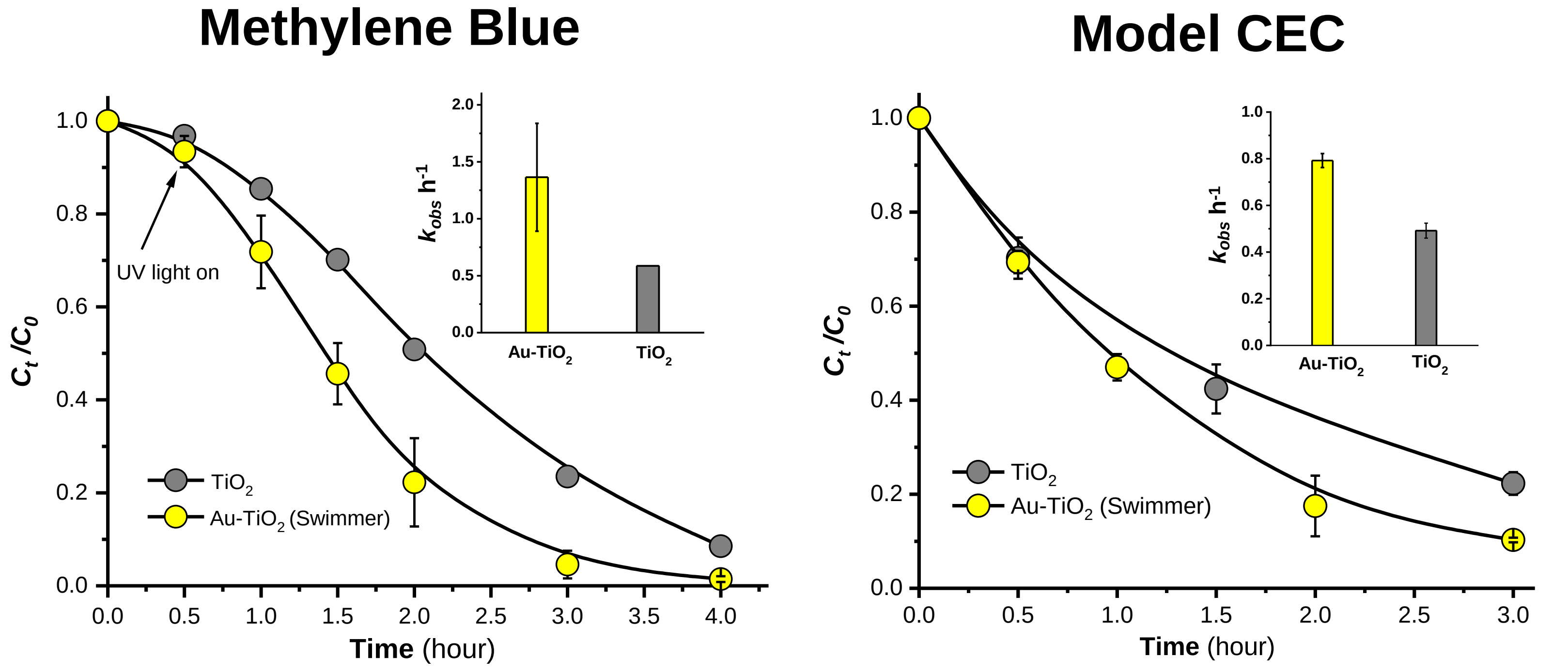


Figure 2: Degradation of (a) methylene blue, validating previous results [3], and (b) a model CEC using Au-TiO_2 micromotors. Inset shows effective degradation rate constants for each case. **Take-home message: Au/TiO_2 micromotors outperform conventional TiO_2 nanoparticles, potentially enabling more efficient and economical pollutant degradation using AOPs.**

FINITE-ELEMENT SIMULATIONS

The micromotors propel themselves in water by self-electrophoresis [2]. We conducted finite-element simulations of self-propulsion and contaminant degradation by the micromotors.

Swimming Speed

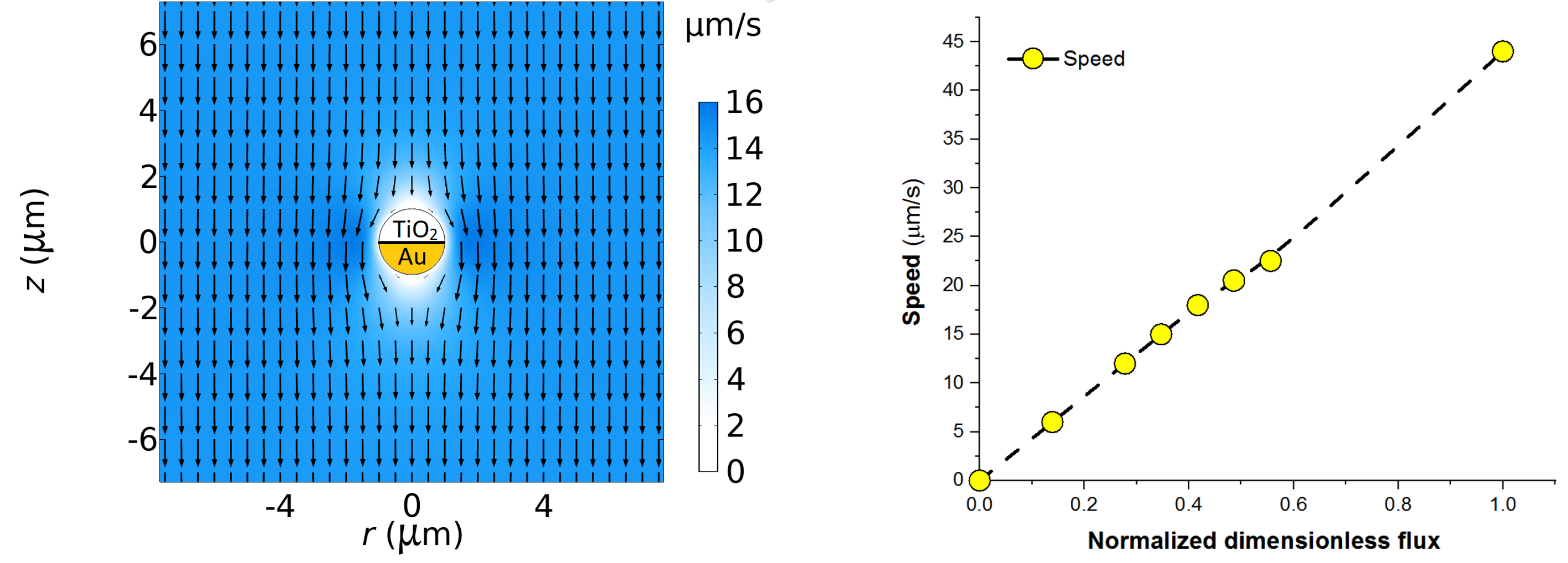


Figure 3: Results of simulations (using COMSOL) of micromotor self-propulsion. (a) Velocity field of aqueous solution in the micromotor reference frame. (b) Self-propelled speed increases with rate of the surface reactions depicted in Figure 1; this reaction rate is proportional to UV light intensity. **Take-home message: simulations accurately replicate dependence of speed on reaction rate.**

Pollutant Concentration

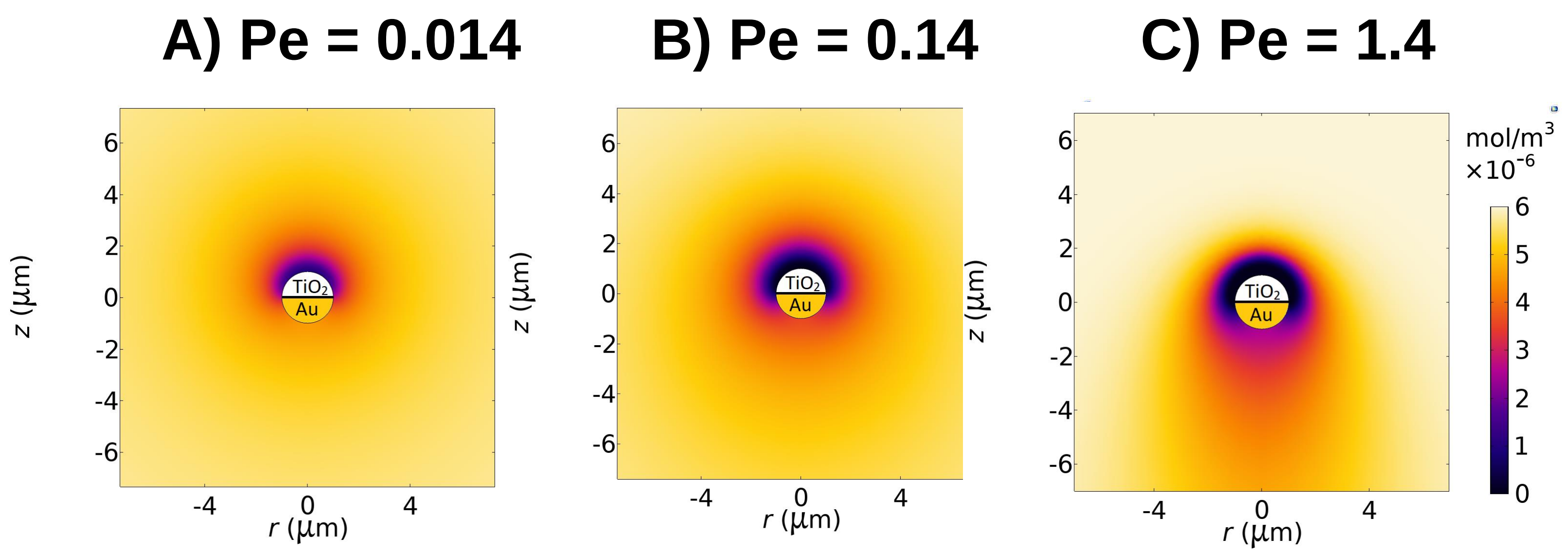


Figure 4: Contaminant concentration distribution for three different Péclet numbers ($Pe = Ud/D$, where U is micromotor speed, d is its diameter, D is pollutant diffusivity). Varying Pe models variations in speed, particle size, and type of pollutant. **Take-home message: as Pe increases, motion alters contaminant distribution more strongly.**

CONCLUSIONS

- Au/TiO_2 micromotors accelerate degradation of methylene blue and a model CEC
- Potential mechanisms of degradation enhancement: (1) convective transport of pollutant due to swimming-generated fluid mixing, (2) enhanced photocatalysis (e.g. presence of Schottky barrier, increased quantum efficiency)

FUTURE WORK

- Compare degradation performance with P25 TiO_2 (widely-accepted industry benchmark for photocatalytic AOPs)
- Explore magnetic control [1,3] and collection after treatment
- Explore using Ag, Cu, Pt instead of Au [4]

APPENDIX: GOVERNING EQUATIONS

Poisson's equation for electric potential V

$$-\epsilon\nabla^2 V = F\Sigma_i z_i c_i = \rho_f$$

Navier-Stokes equation for velocity $\boldsymbol{u}$

$$\rho\frac{\partial}{\partial t}\boldsymbol{u} + \rho(\boldsymbol{u}\cdot\nabla\boldsymbol{u}) = -\nabla p + \eta\nabla^2\boldsymbol{u} - \rho_f\nabla V$$

Convection-diffusion equation for species concentration c_i

$$\frac{\partial c_i}{\partial t} = \nabla\cdot(D_\mathrm{i}\nabla c_i) - \boldsymbol{u}\cdot\nabla c_i + z_i F c_i \mu_i \nabla V + \Sigma R_{ij}$$

in which the reaction rate R_{ij} between species i and j is

$$R_{ij} = -\frac{\partial c_i}{\partial t} = -\frac{\partial c_j}{\partial t} = -k_{ij}c_i c_j$$

Symbols meanings are as follows: ϵ (permittivity of medium) [F/m] , F (Faraday's constant) [C/mol], z_i (valence of species i), ρ_f (charge density) [C/m^3], D_i (diffusivity of species i) [m^2/s], μ_i(mobility of species i) [s/mol·kg], ρ (fluid density) [kg/m^3], p (fluid pressure) [N/m^2], η (dynamic viscosity) [N·s/m^2], k_{ij} (reaction rate constant between i and j) [m^3/mol·s]

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