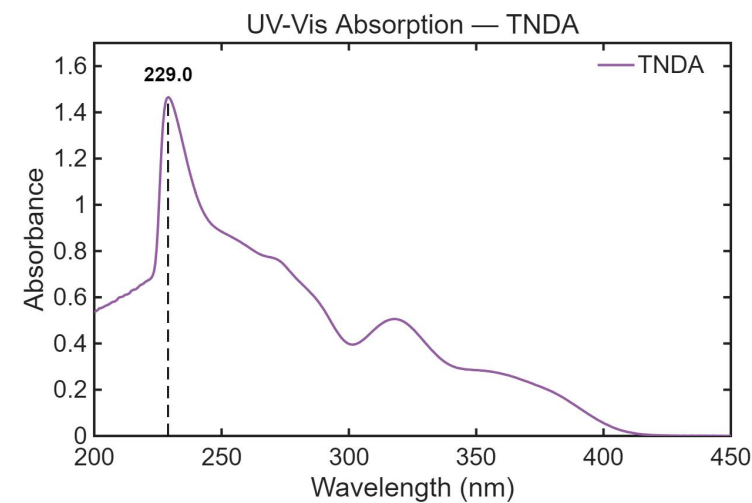
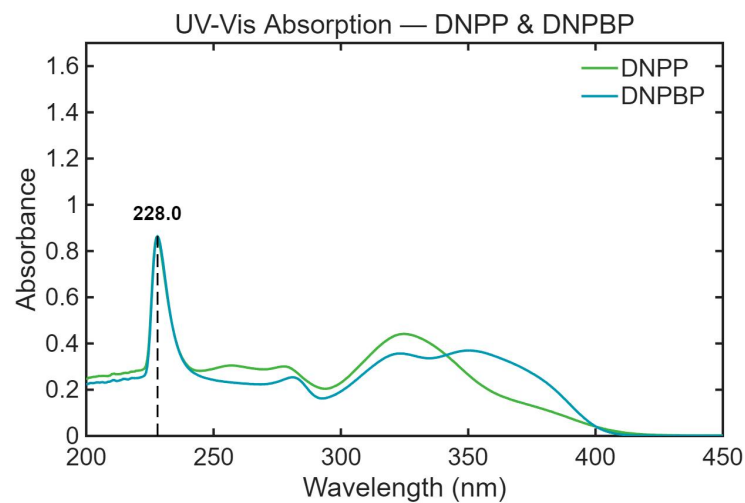
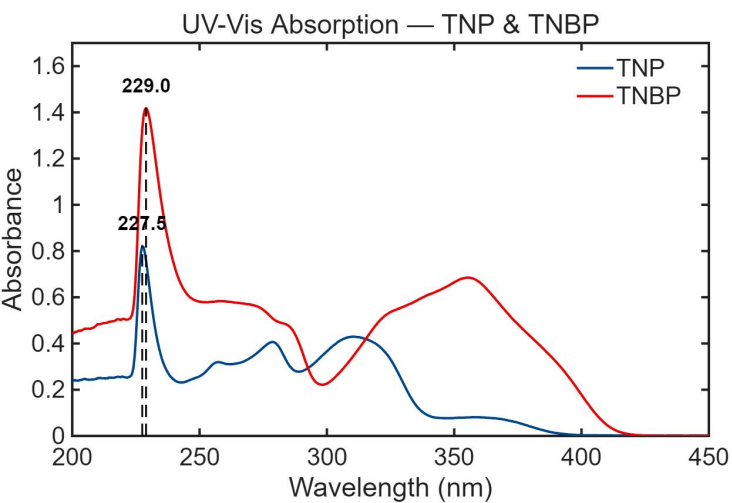
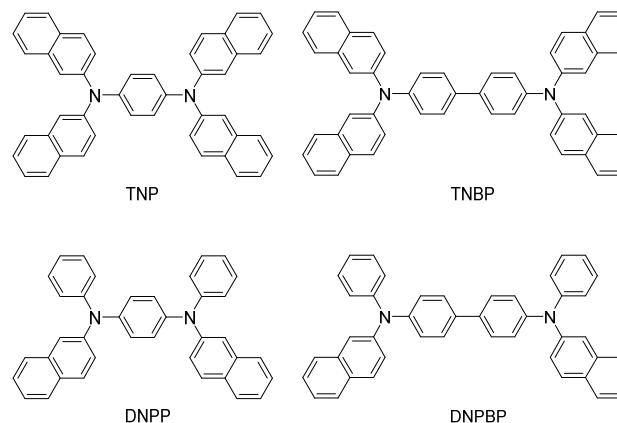
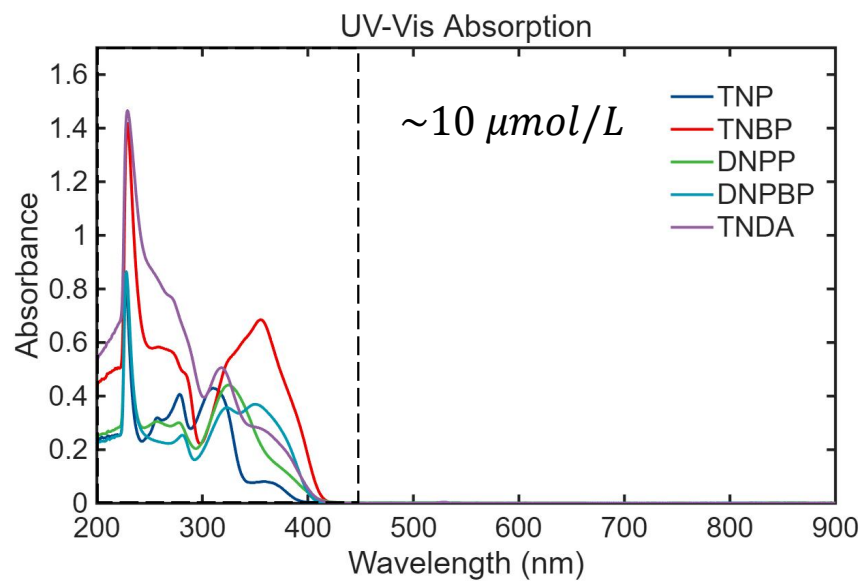


UV-vis CSSample



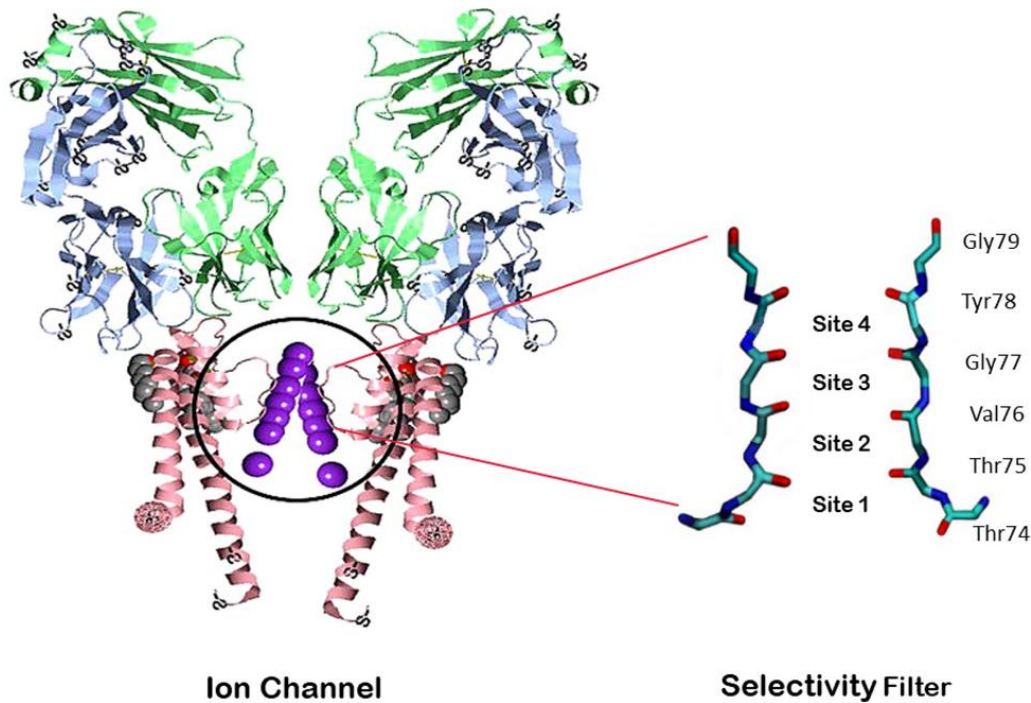


Quantum Ion Coherence in Biological Ion Channels

2026.08.24

汇报人: 郑民熙

Introduction



A. Quantum coherence on selectivity and transport of ion channels. *Sci Rep* **12**, 9237 (2022).

KcsA

Potassium channel with high selectivity and flux

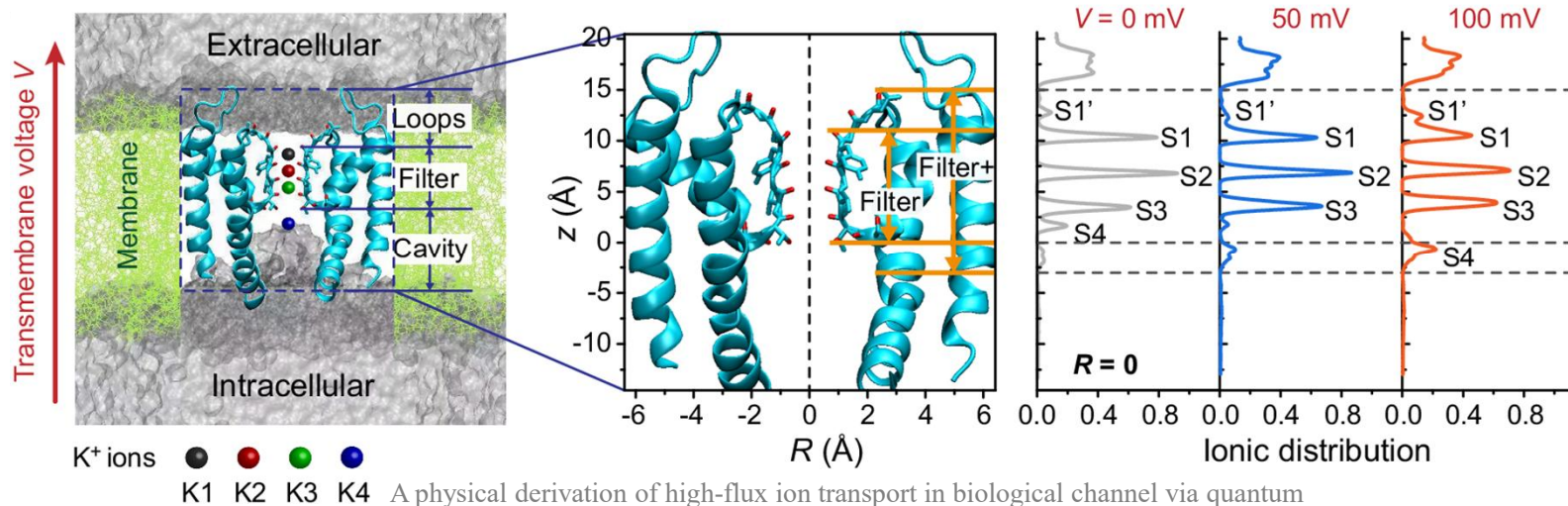
Reasons:

- Precise coordination by the selectivity filter (TVGYG)
- Size match between the channel and K^+
- **“Knock-on” mechanisms – interactions between K^+ in different sites.**

Multi-ion interactions $\leftrightarrow$ Quantum Coherence?

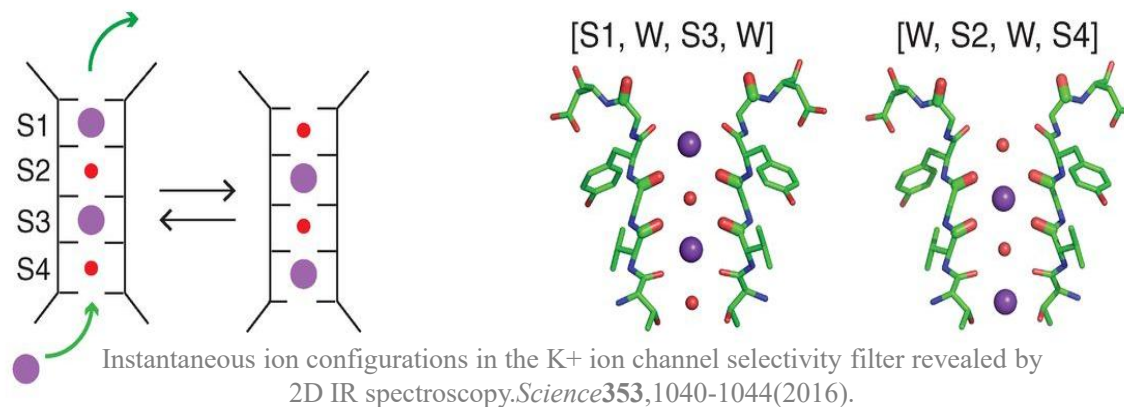
Transportation

Hard-knock model



A physical derivation of high-flux ion transport in biological channel via quantum ion coherence. *Nat Commun* **15**, 7189 (2024).

Knock-on model



Hard-knock Model

MD simulation

ion coherence order degree α_{F+}/α_F

$$\alpha_{F+}(t) = A_n \sum_{i<j}^N f(v_{ij}^{\rightarrow})$$

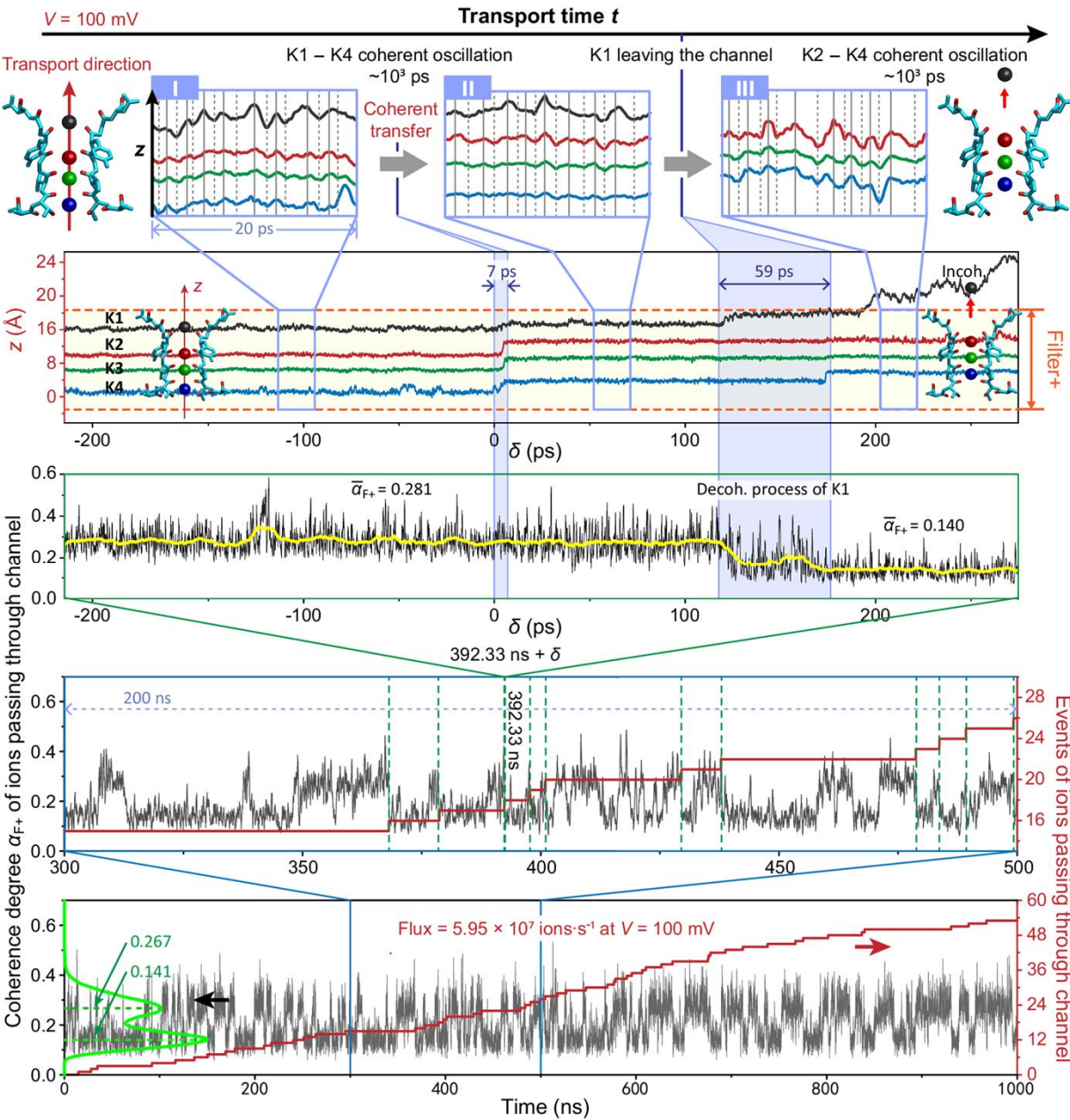
$$\alpha_F(t) = B_n \sum_{i<j}^N f(v_{ij}^{\rightarrow})$$

$$f(v_{ij}^{\rightarrow}) = 1 - \frac{|v_i^{\rightarrow} - v_j^{\rightarrow}|}{|v_i^{\rightarrow}| + |v_j^{\rightarrow}|}$$

$$A_n = \binom{n_{all\ ions}}{2} \quad B_n = \binom{n_{ions\ inside\ the\ tunnel}}{2}$$

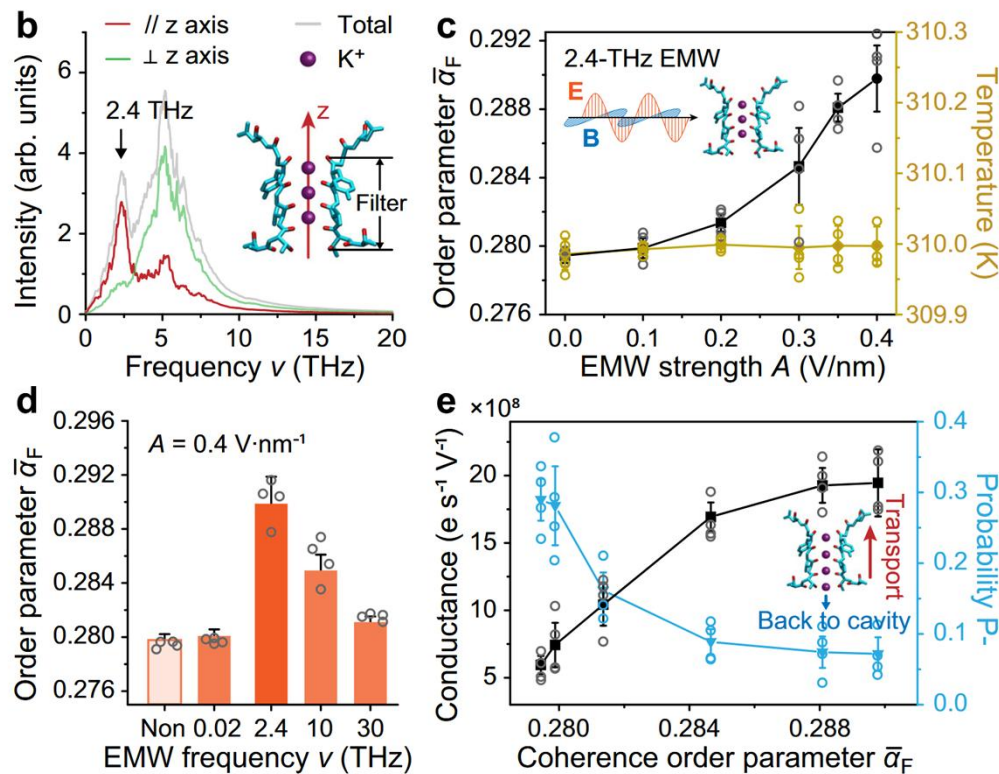
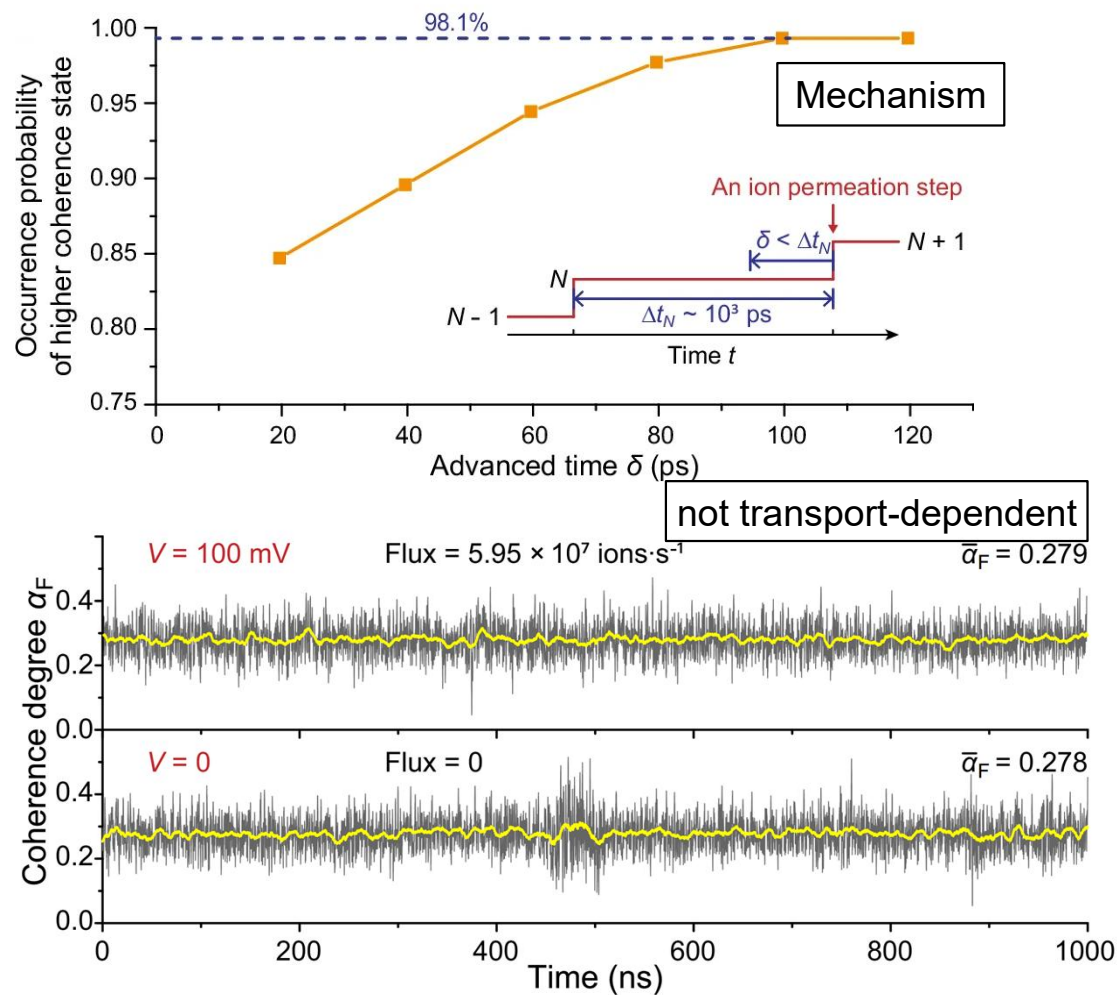
A physical derivation of high-flux ion transport in biological channel via quantum ion coherence. *Nat Commun* **15**, 7189 (2024).

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Hard-knock Model

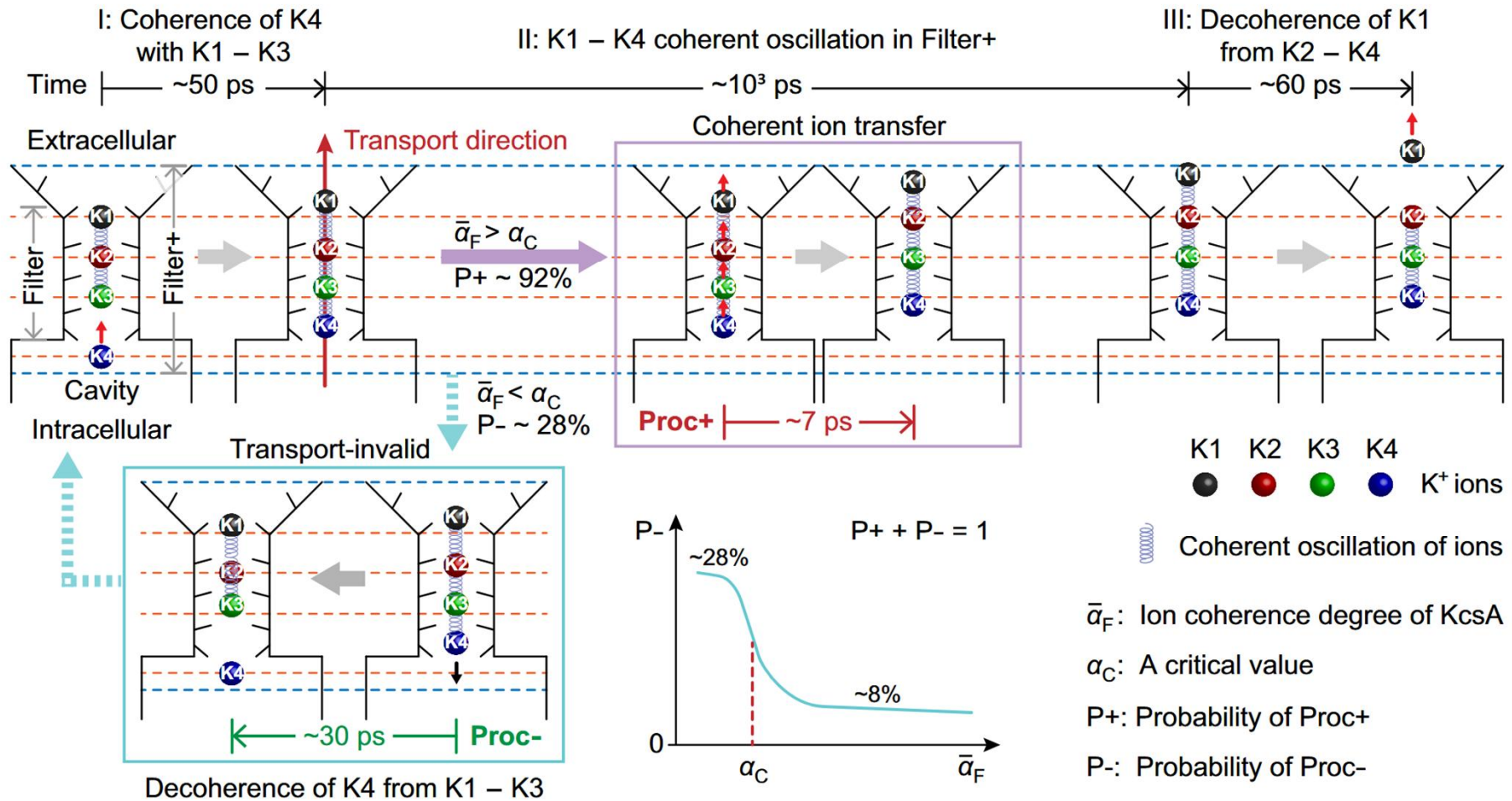
Further Analyses



Ion flux positively associated with the intrinsic ion coherence α_F

Hard-knock Model

Conclusion



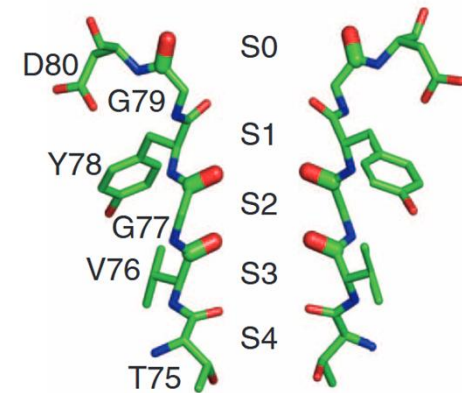
Knock-on Model

Verifications

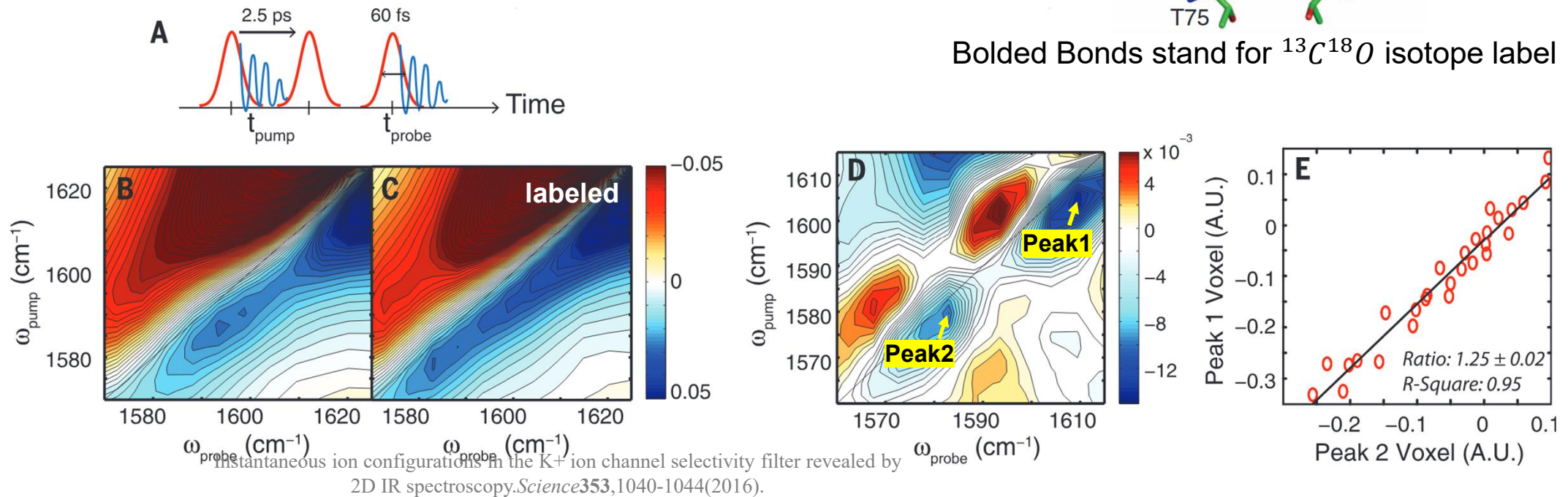


The pulse sequence produces an infrared signal that oscillates as a function of the time delay between the pump pulses and after the probe pulse, respectively. The signal is Fourier transformed along these two time axes to give a 2D IR spectrum that correlates the two frequency axes.

For each isotope label, the pulse sequence will create a pair of oppositely signed peaks, with the negative peak on the diagonal.



Bolded Bonds stand for $^{13}\text{C}^{18}\text{O}$ isotope label

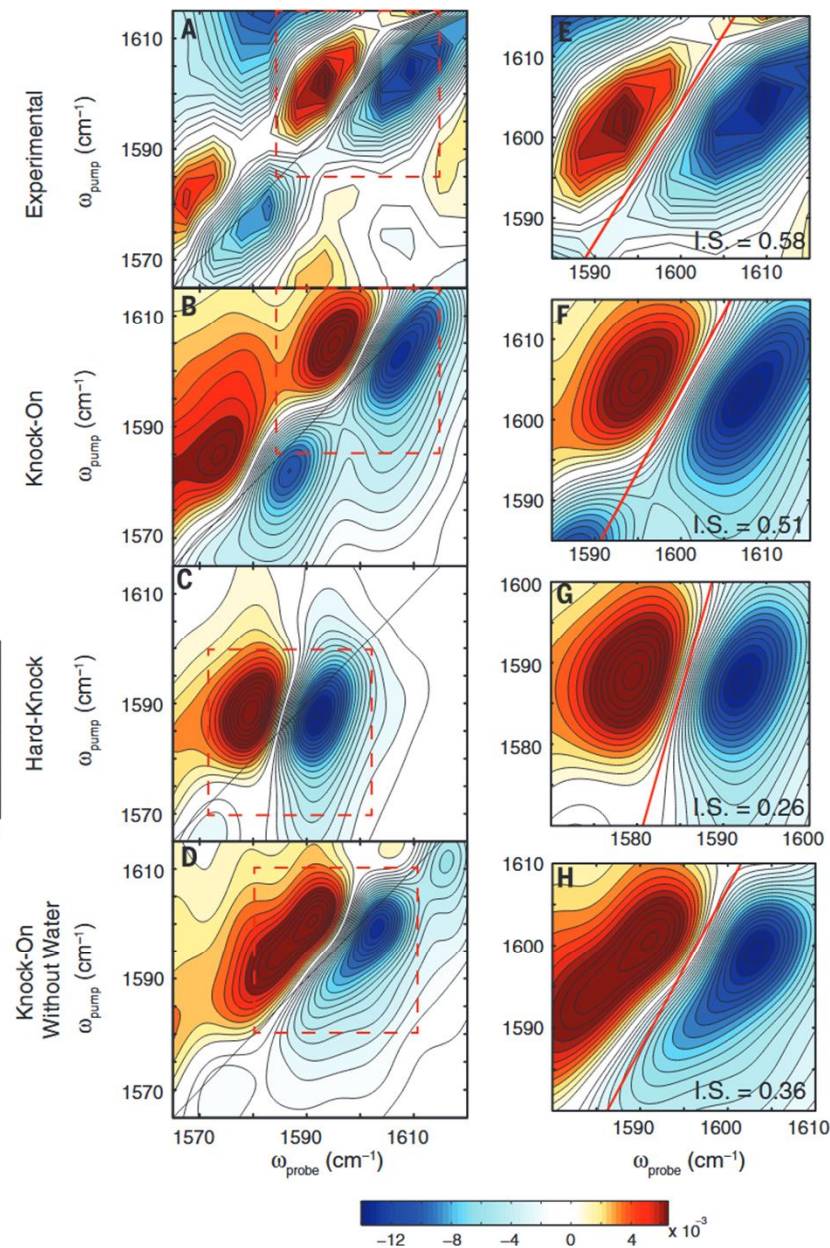
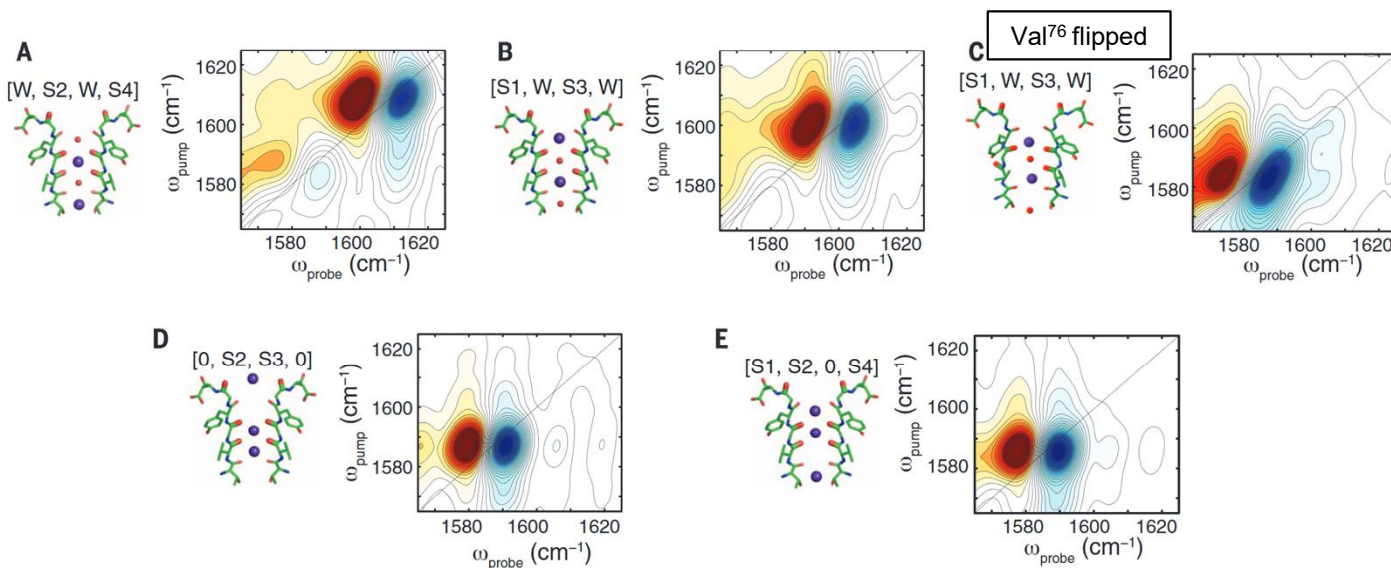


Knock-on Model

Verifications

MD calculations:

- Weight average of different ion-binding states.
 - 30% **A**+30% **B**+40% **C**
- The temporal resolution of 2D IR spectroscopy is orders of magnitude shorter than the time scales for ion permeation.
- Hence we can determine from the 2D IR spectra the relative populations of each of these ion-binding states by the peaks.



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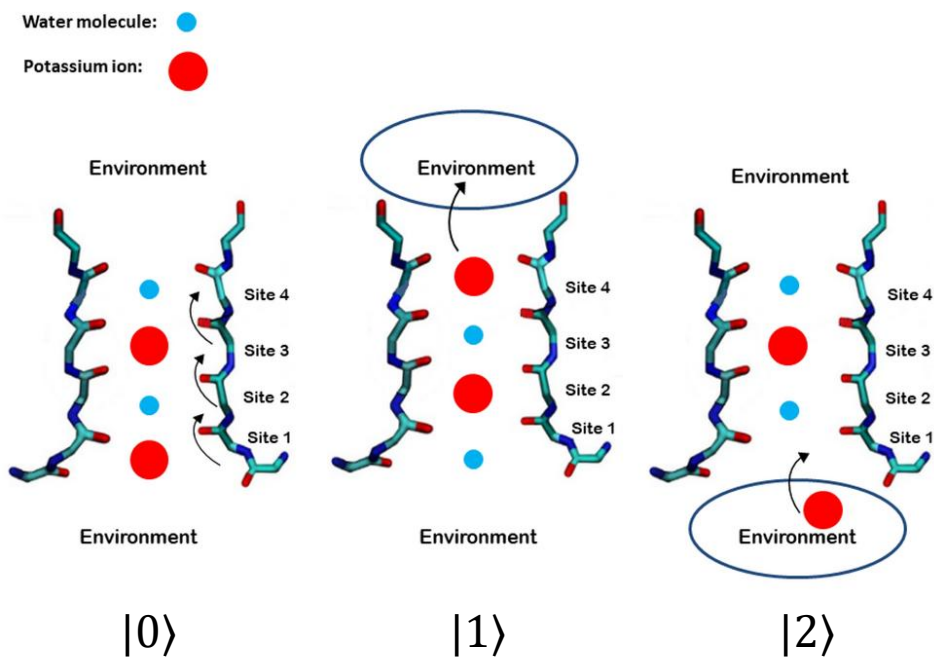
Instantaneous ion configurations in the K⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. *Science* **353**,1040-1044(2016).

Knock-on Model

Starting with the superposition of:

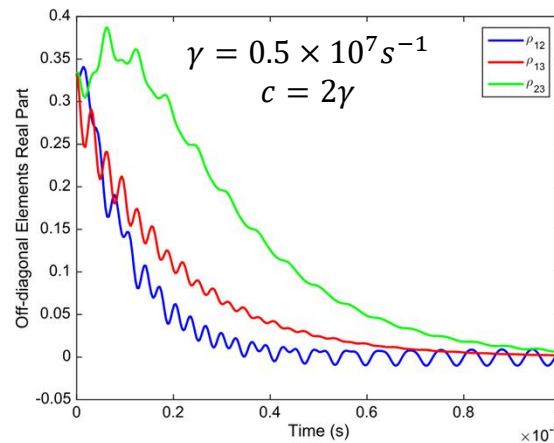
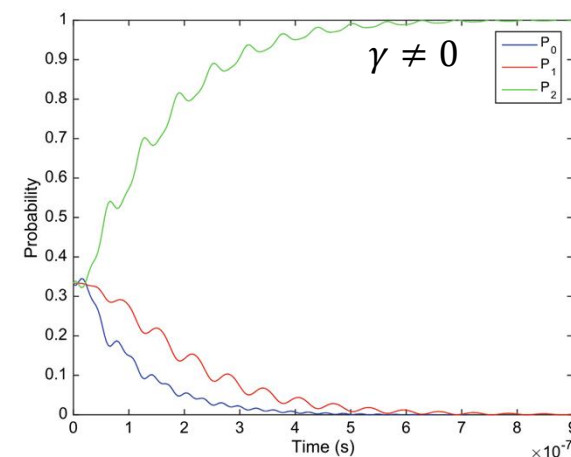
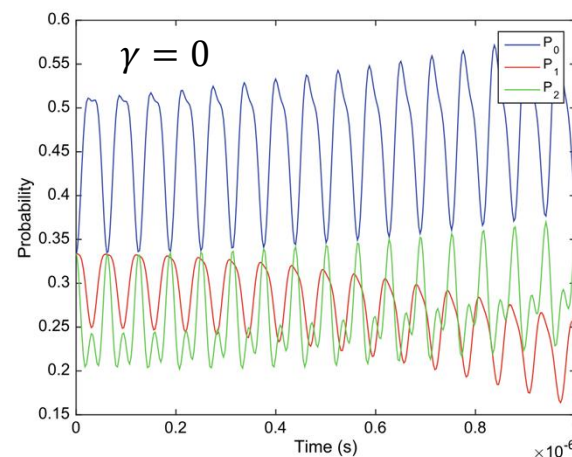
$$|\varphi\rangle = \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + |2\rangle)$$

Within the Lindblad equation with decoherent rate γ and hopping rate c

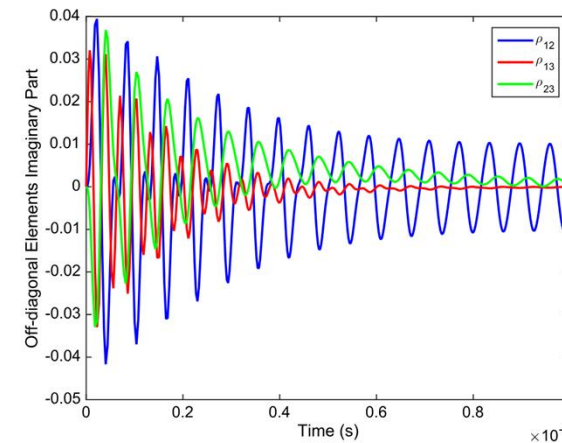


Quantum coherence on selectivity and transport of ion channels. *Sci Rep* **12**, 9237 (2022).

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(a)



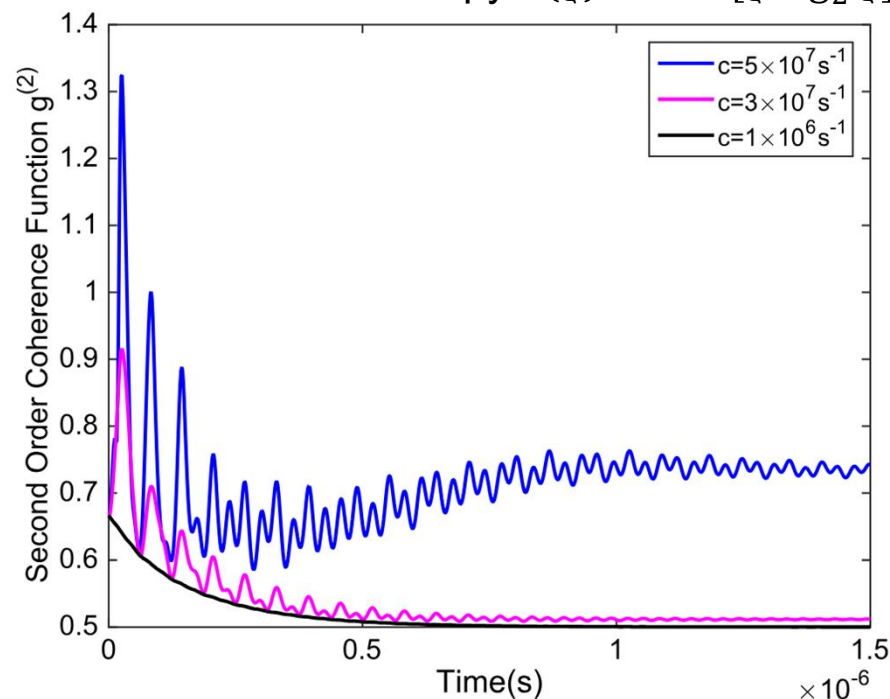
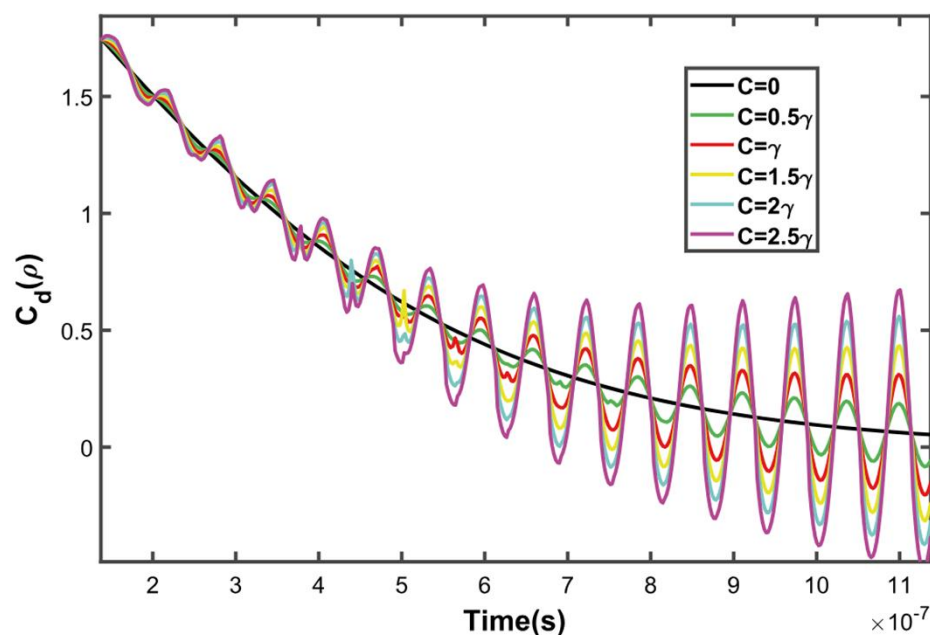
(b)

Knock-on Model

Distillable Coherence $C_d(\rho)$:

$$C_d(\hat{\rho}) = S(\Delta[\hat{\rho}]) - S(\hat{\rho})$$

with $\Delta[\hat{\rho}] = \sum_{i=0}^{d-1} |i\rangle\langle i| \hat{\rho} |i\rangle\langle i|$ as an dephasing operator and Von Neumann entropy $S(\hat{\rho}) = -\text{Tr}[\hat{\rho} \log_2 \hat{\rho}]$



Quantum coherence on selectivity and transport of ion channels. *Sci Rep* **12**, 9237 (2022).

Coherence maintained in high hopping (high flux) channels

Conclusion



The two primary transport mechanisms proposed for the KcsA channel—namely, the hard-knock and knock-on models—have yet to be rigorously validated. Notably, quantum coherence has been invoked in both frameworks to account for the channel's paradoxical combination of high selectivity and high flux. Therefore, obtaining direct experimental evidence of quantum coherence within this system is crucial for elucidating and verifying the underlying transport dynamics.