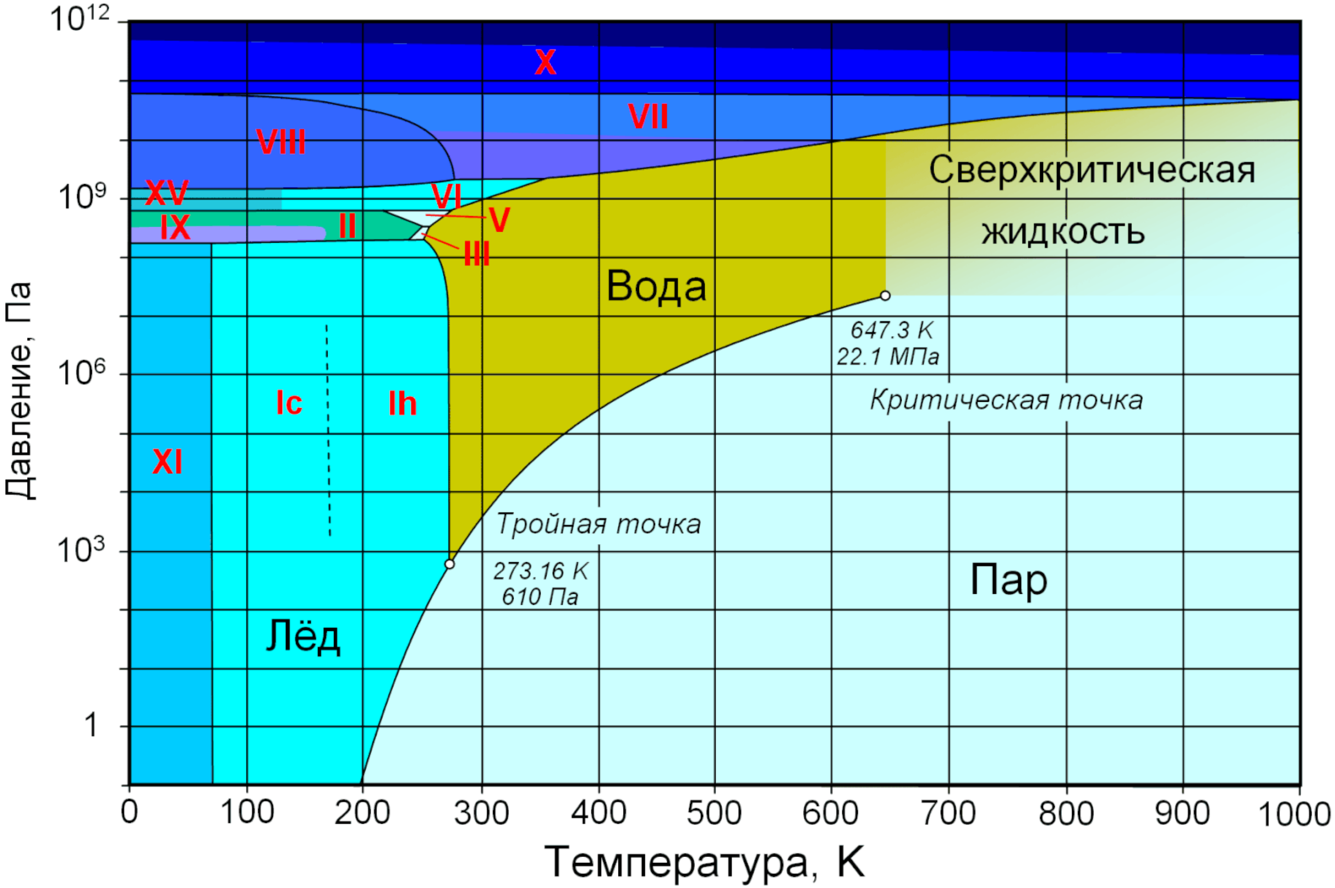
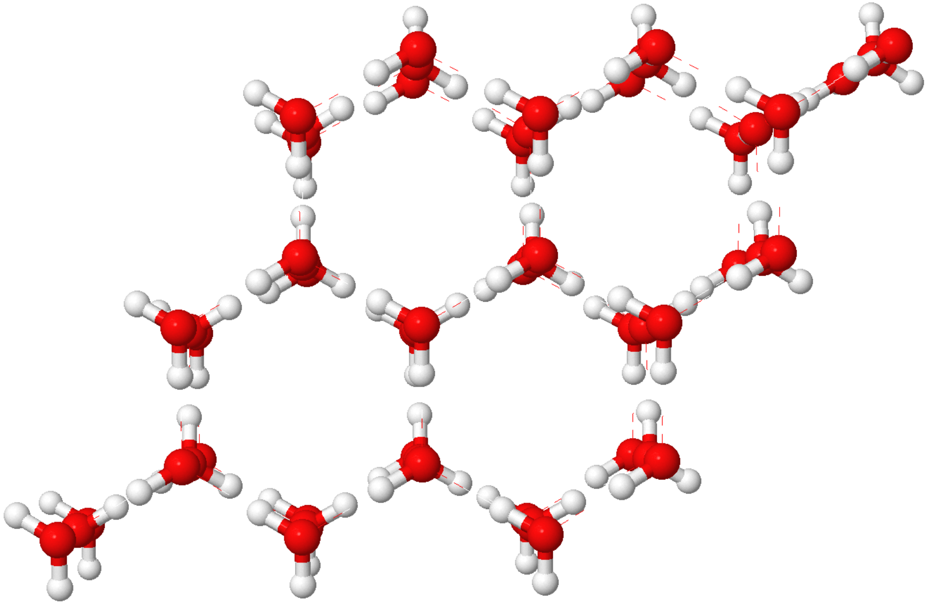
Quantum Phase Transition in the One-Dimensional Water Chain

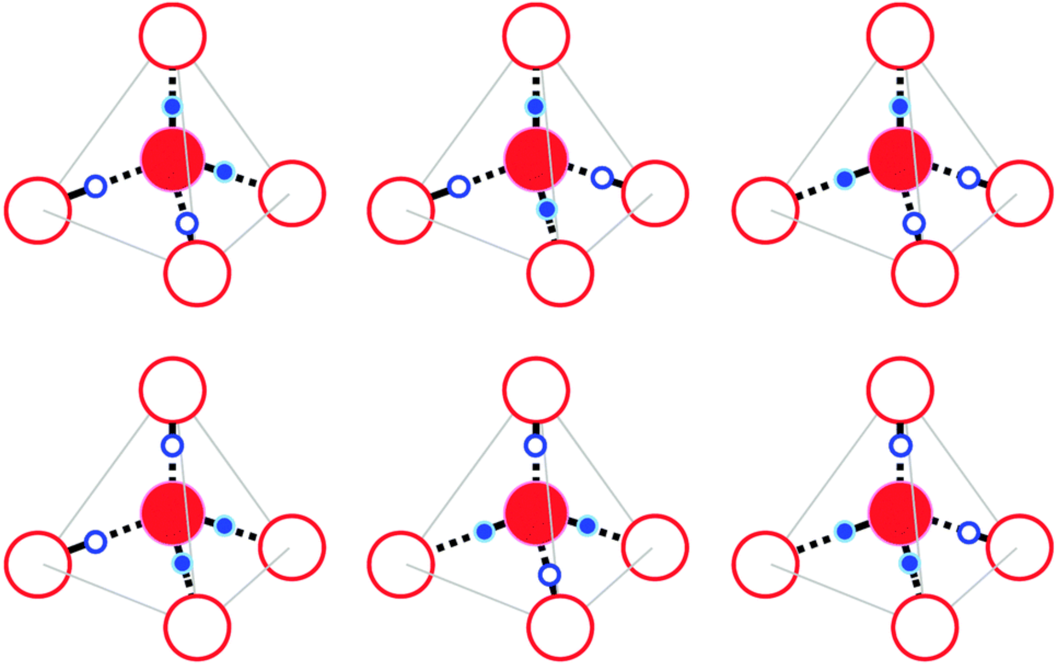
T. Serwatka, R.G. Melko, A. Burkov, and P.-N. Roy,
Phys. Rev. Lett. 130, 026201 (2023)

Ice

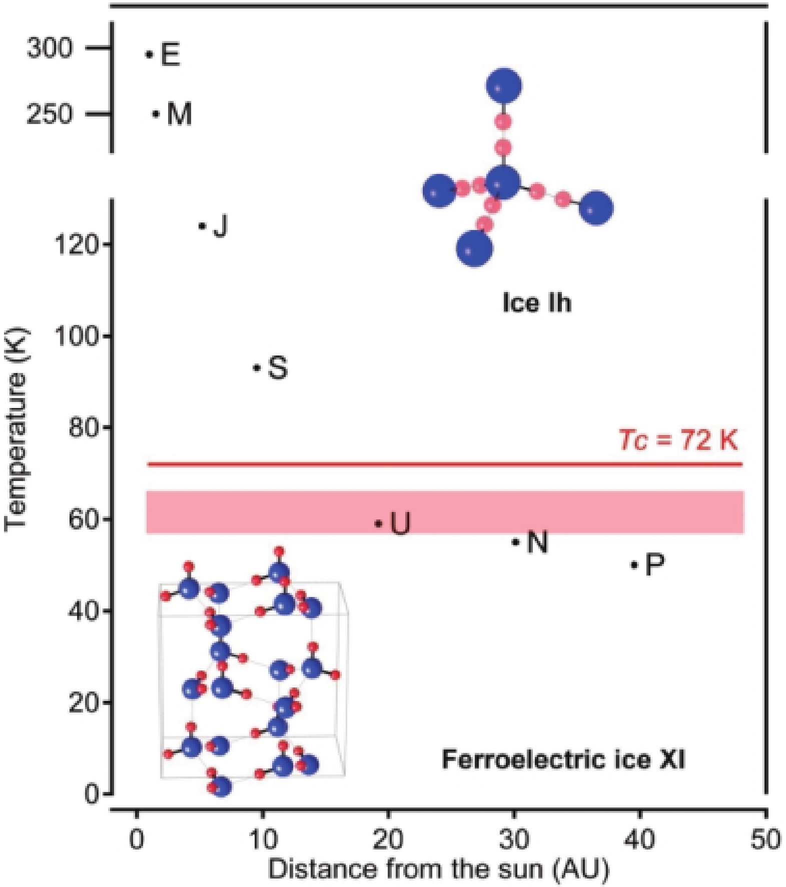

X
VII
VIII
XV
VI
V
IX
II
III
Сверхкритическая жидкость
Вода
647.3 K
22.1 МПа
Критическая точка
Ic
Ih
XI
Тройная точка
273.16 K
610 Па
Пар
Лёд
10^{12}
10^9
10^6
10^3
1
Давление, Па
0
100
200
300
400
500
600
700
800
900
1000
Температура, К

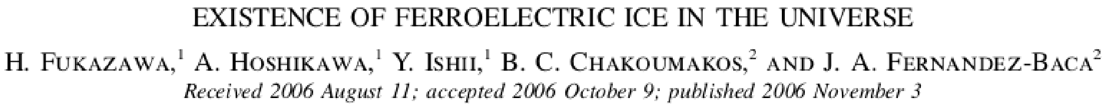
Hexagonal ice





Ferroelectric ice




EXISTENCE OF FERROELECTRIC ICE IN THE UNIVERSE

H. Fukazawa,[1] A. Hoshikawa,[1] Y. Ishii,[1] B. C. Chakoumakos,[2] and J. A. Fernandez-Baca[2]

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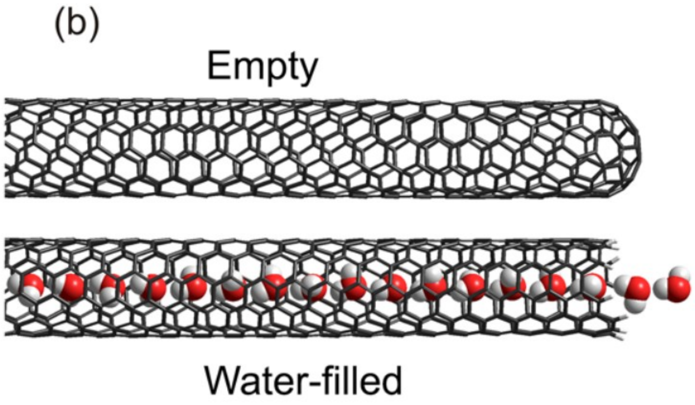
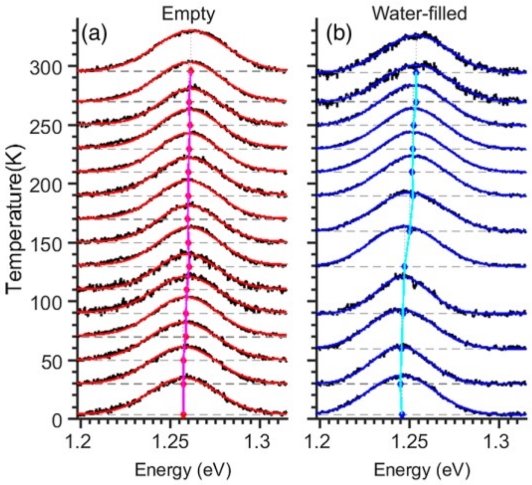
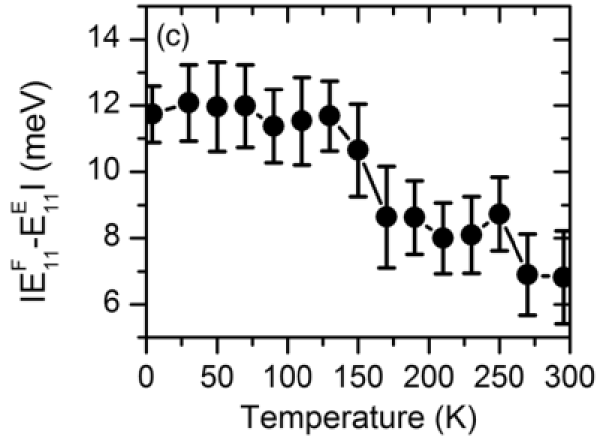
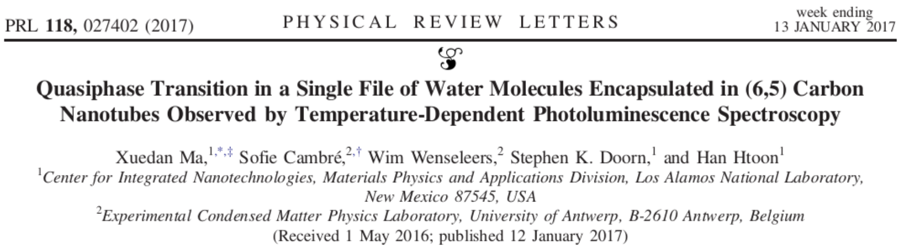
Water in porous channels









PRL **118,** 027402 (2017) PHYSICAL REVIEW LETTERS week ending 13 JANUARY 2017

Quasiphase Transition in a Single File of Water Molecules Encapsulated in (6,5) Carbon Nanotubes Observed by Temperature-Dependent Photoluminescence Spectroscopy

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Water in porous channels

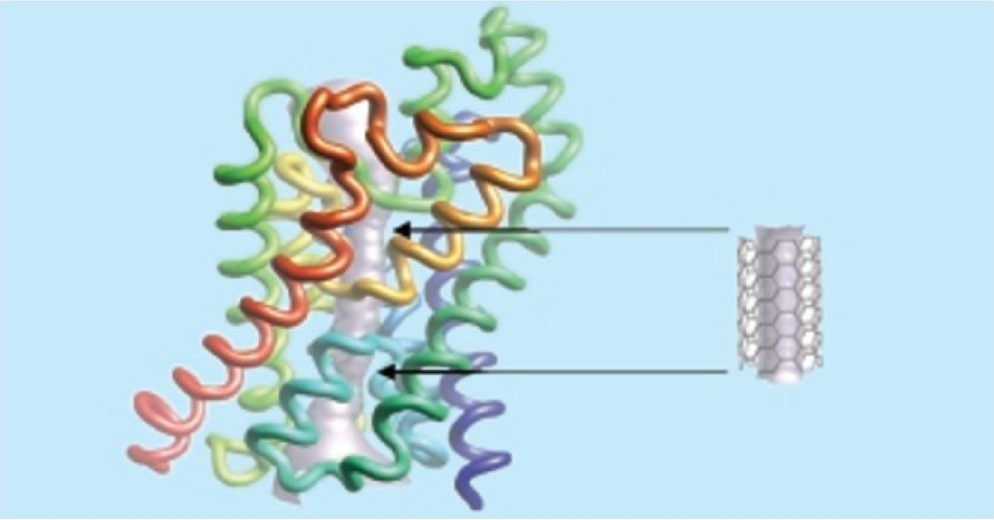

Figure 1 **Pore comparisons. Left, a biological pore (grey), as found in the bacterial water and glycerol channel, GlpF. The pore is formed by the side chains of the protein backbone (seen here as coloured spaghetti). Right, a similar pore in a narrow carbon nanotube, such as that for which Hummer *et al.*[1] carried out simulations of water conduction. It is hoped that nanotubes can be used in simulations**

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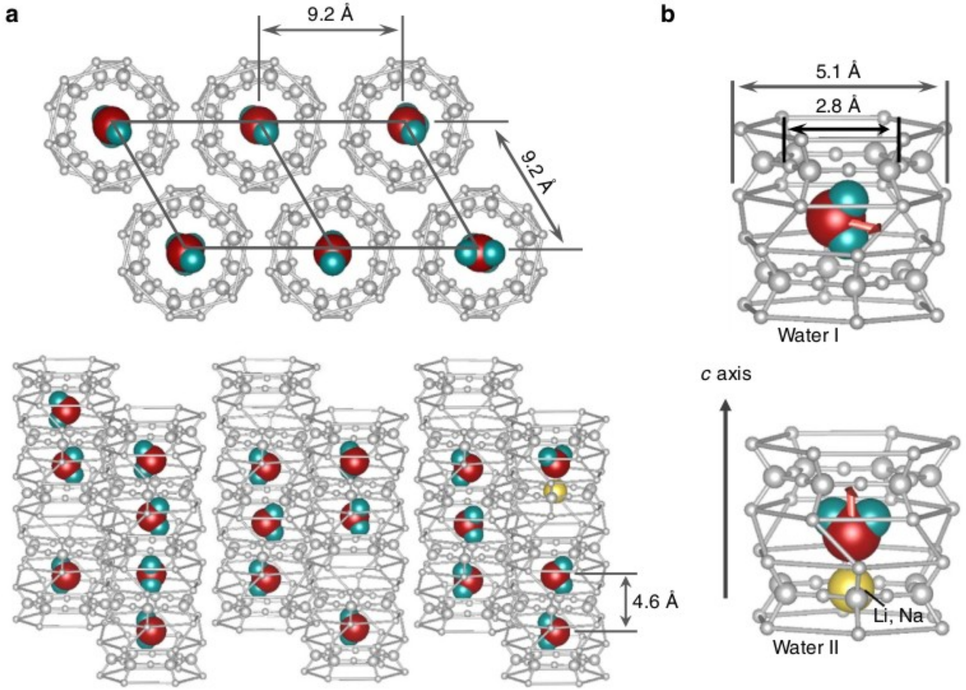
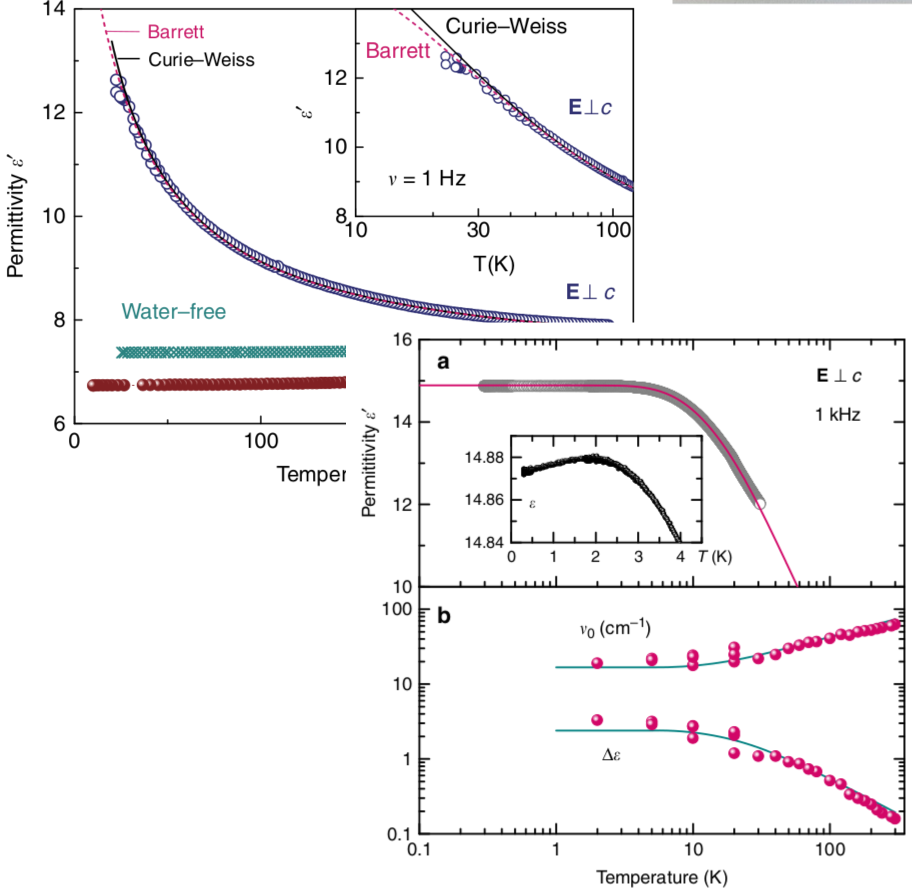
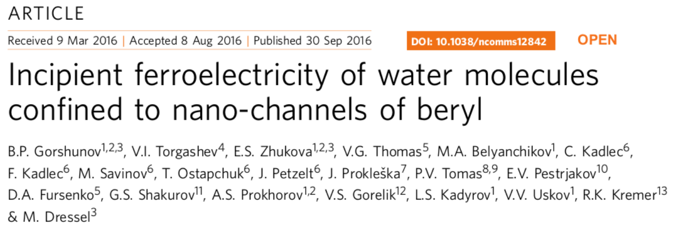
Water in porous channels






ARTICLE

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Incipient ferroelectricity of water molecules confined to nano-channels of beryl

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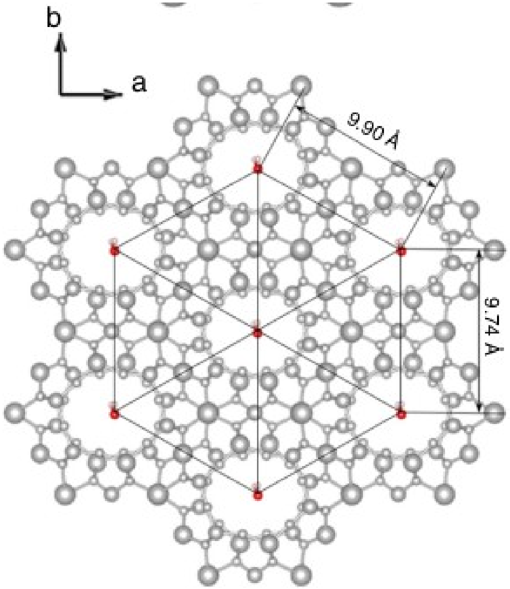
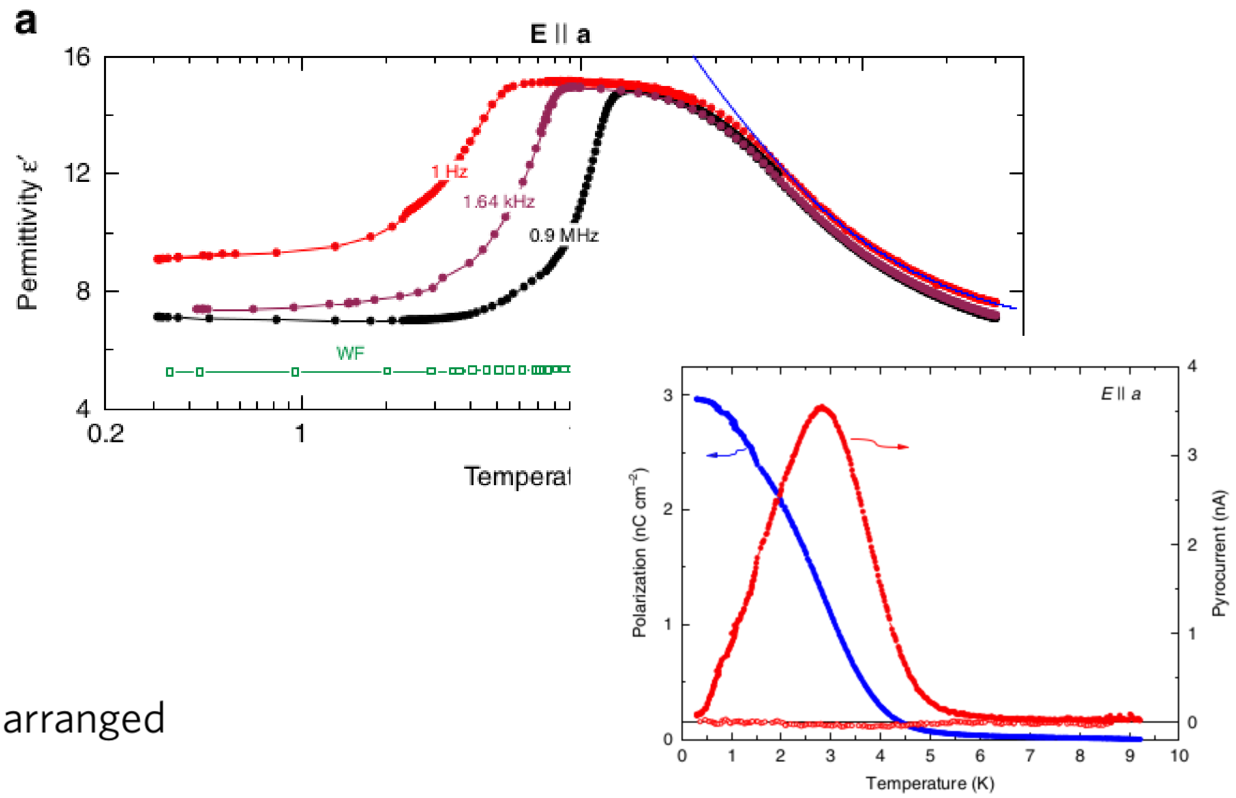
Water in porous channels





https://doi.org/10.1038/s41467-020-17832-y **OPEN**

Dielectric ordering of water molecules arranged in a dipolar lattice

M. A. Belyanchikov[1✉], M. Savinov[2], Z. V. Bedran[1], P. Bednyakov[2], P. Proschek[3], J. Prokleska[3], V. A. Abalmasov[4], J. Petzelt[2], E. S. Zhukova[1], V. G. Thomas[5,6], A. Dudka[7], A. Zhugayevych[8], A. S. Prokhorov[1,9], V. B. Anzin[1,9], R. K. Kremer[10], J. K. H. Fischer[11,12], P. Lunkenheimer[11], A. Loidl[11], E. Uykur[13], M. Dressel[1,13] & B. Gorshunov[1✉]

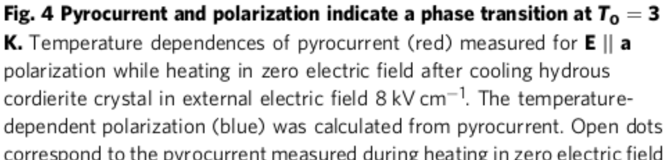
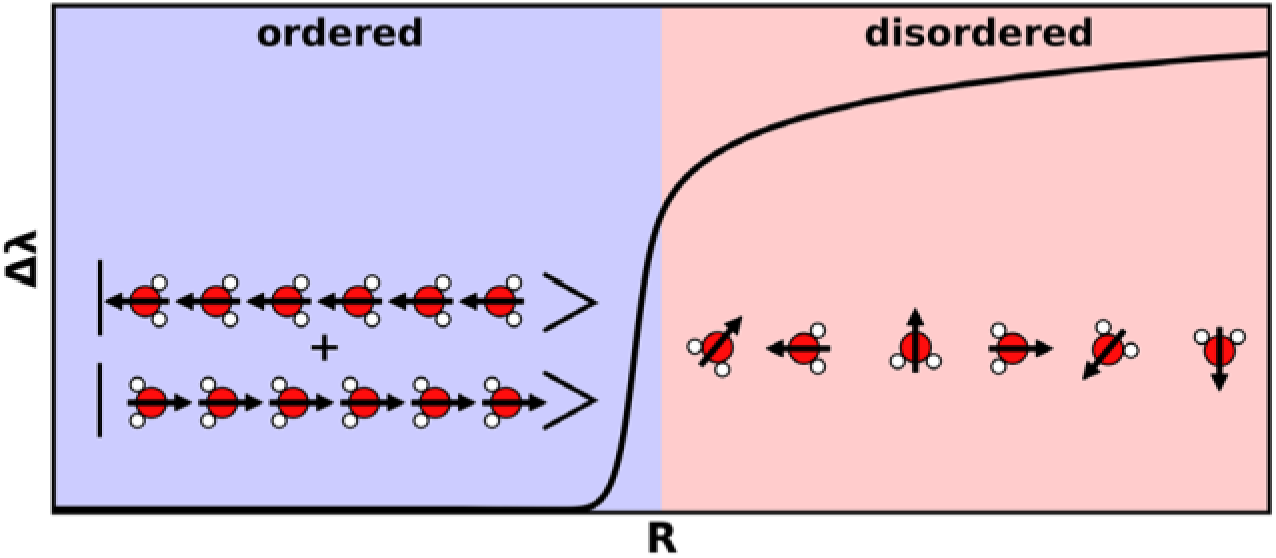


Fig. 4 Pyrocurrent and polarization indicate a phase transition at $T_0 = 3$ K. Temperature dependences of pyrocurrent (red) measured for **E** || **a** polarization while heating in zero electric field after cooling hydrous cordierite crystal in external electric field 8 kV cm^{-1}. The temperature-dependent polarization (blue) was calculated from pyrocurrent. Open dots correspond to the pyrocurrent measured during heating in zero electric field

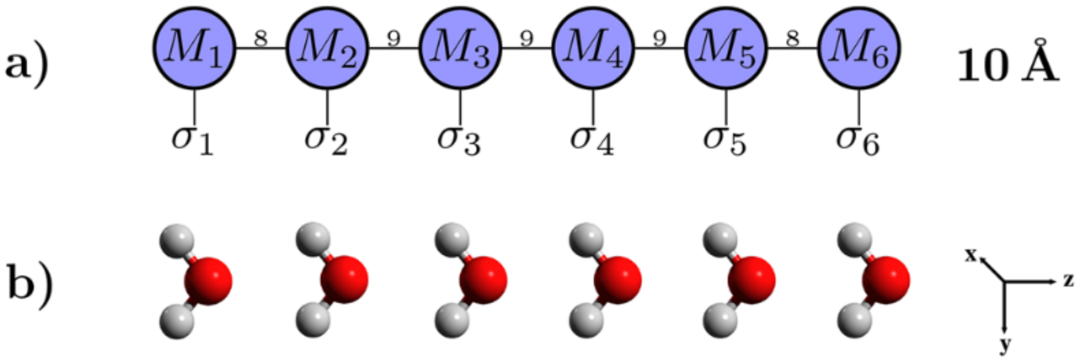
Phase transition simulation



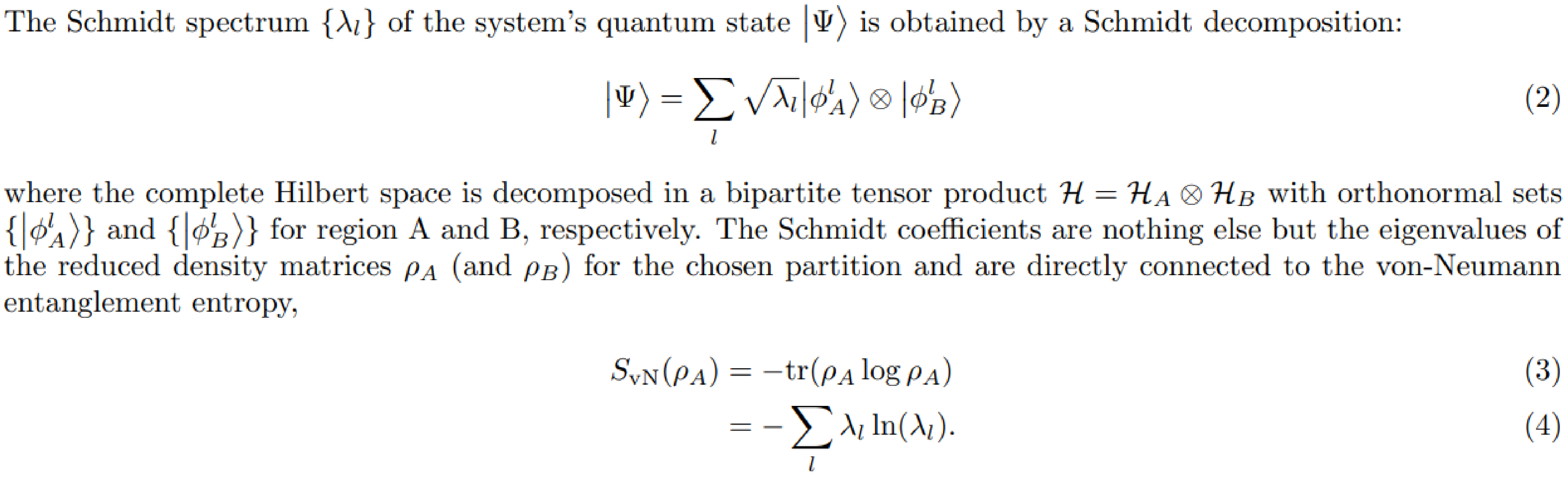
Computational details

$$|\Psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} C_{\sigma_1,\ldots,\sigma_N} |\sigma_1 \ldots \sigma_N\rangle,$$

$$\begin{aligned} C_{\sigma_1,\ldots,\sigma_N} &= \sum_{\{\alpha\}} M^{(1),\sigma_1}_{1\alpha_1} M^{(2),\sigma_2}_{\alpha_1\alpha_2} \ldots M^{(N),\sigma_N}_{\alpha_{N-1}1} \\ &= \mathbf{M}^{(1),\sigma_1} \mathbf{M}^{(2),\sigma_2} \ldots \mathbf{M}^{(N),\sigma_N}, \end{aligned}$$



Schmidt values



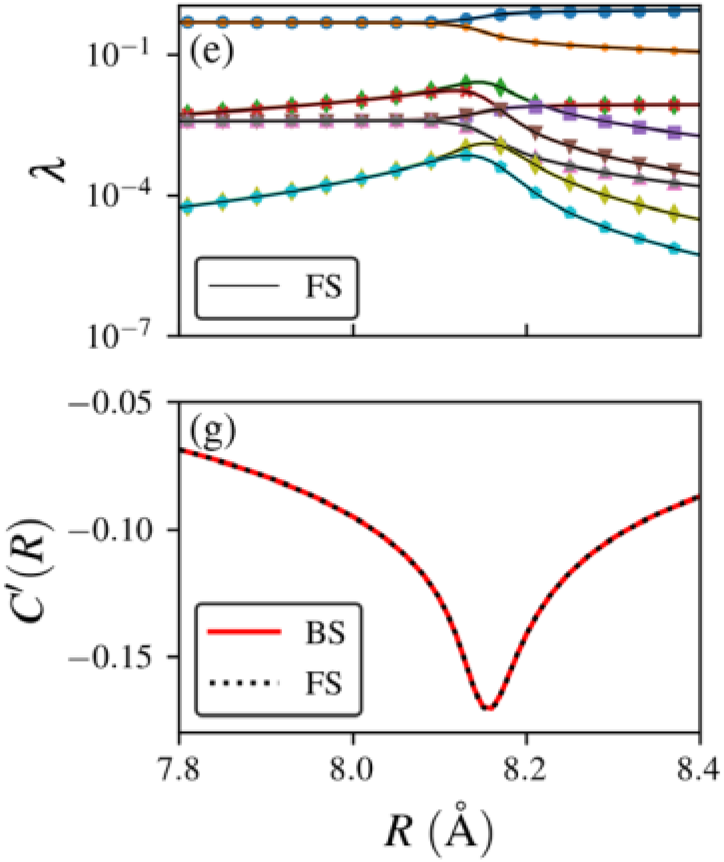
The Schmidt spectrum $\{\lambda_l\}$ of the system's quantum state $\left|\Psi\right\rangle$ is obtained by a Schmidt decomposition:

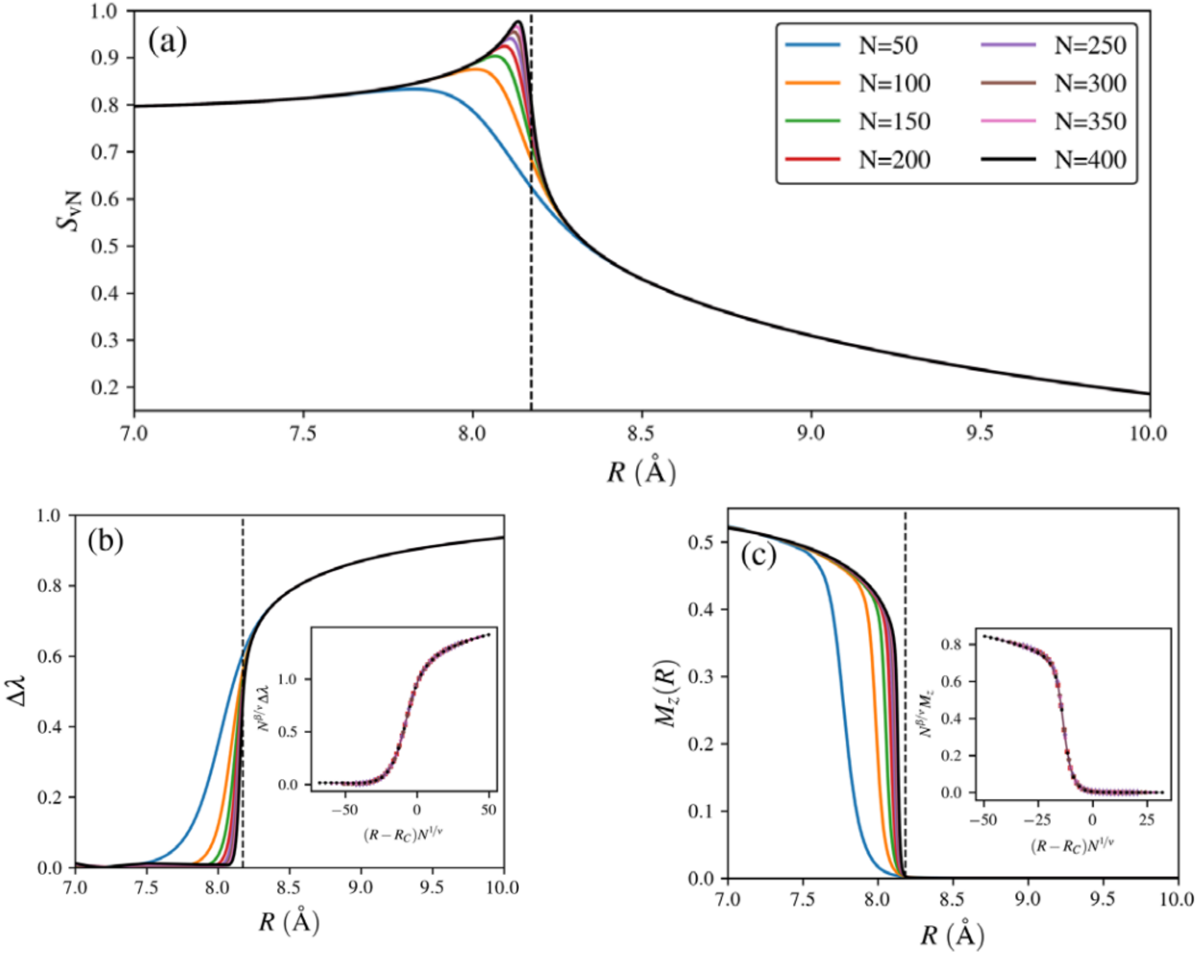
$$\left|\Psi\right\rangle = \sum_l \sqrt{\lambda_l} |\phi_A^l\rangle \otimes \left|\phi_B^l\right\rangle \tag{2}$$

where the complete Hilbert space is decomposed in a bipartite tensor product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with orthonormal sets $\{\left|\phi_A^l\right\rangle\}$ and $\{\left|\phi_B^l\right\rangle\}$ for region A and B, respectively. The Schmidt coefficients are nothing else but the eigenvalues of the reduced density matrices ρ_A (and ρ_B) for the chosen partition and are directly connected to the von-Neumann entanglement entropy,

$$\begin{aligned} S_{\mathrm{vN}}(\rho_A) &= -\mathrm{tr}(\rho_A \log \rho_A) \qquad (3) \\ &= -\sum_l \lambda_l \ln(\lambda_l). \qquad (4) \end{aligned}$$

Quantum phase transition





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