heat transport in water at icy-giants conditions from ab initio MD simulations

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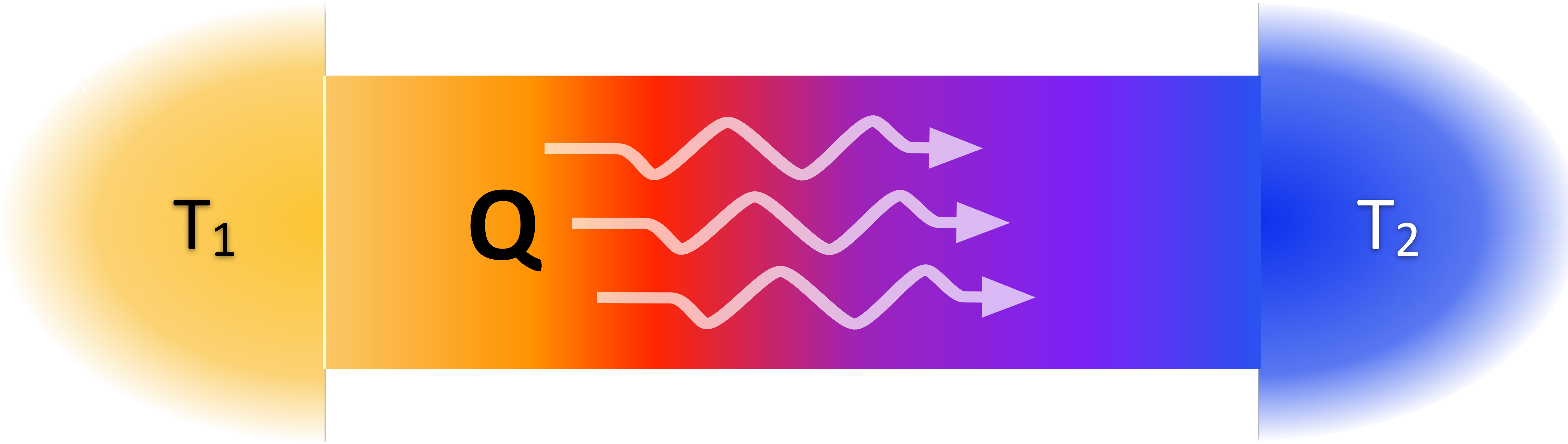
talk given at the *Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie,*
Sorbonne Université, Paris, January 16, 2020

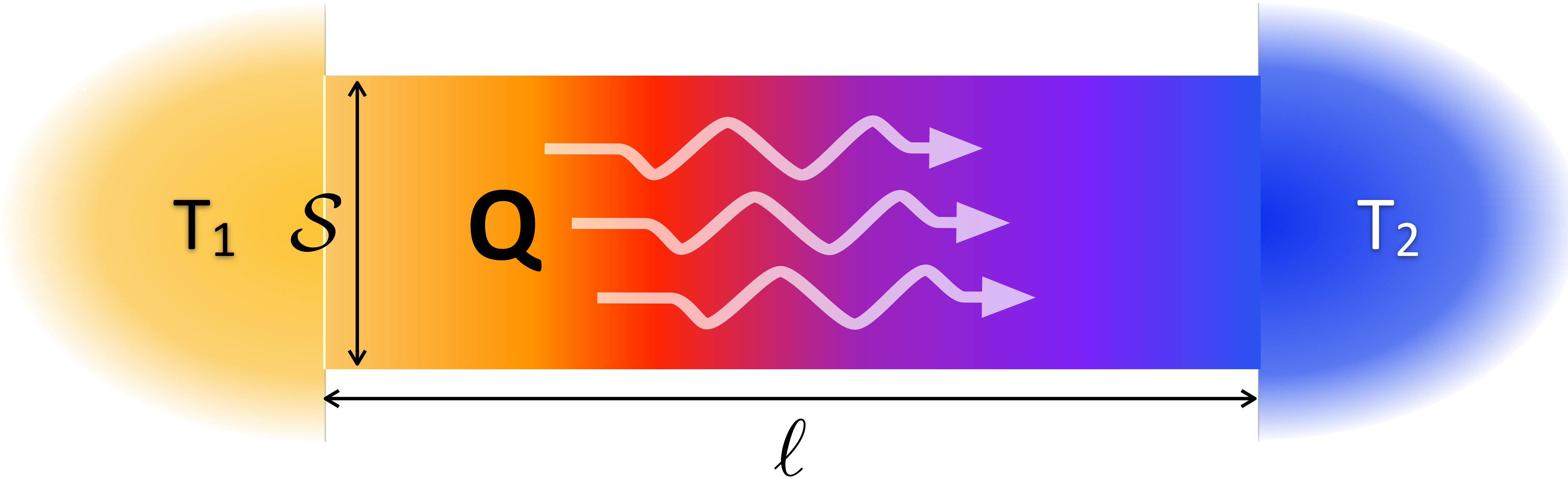
what heat transport is all about



heat flows from the warm to the cool
as time flows from the past to the future

MA PER SEGUIR VIRTUTE E CANOSCENZA

what heat transport is all about



$$\frac{1}{\mathcal{S}}\frac{\mathrm{dQ}}{\mathrm{dt}} = -\kappa\frac{(\mathrm{T}_2 - \mathrm{T}_1)}{\ell}$$

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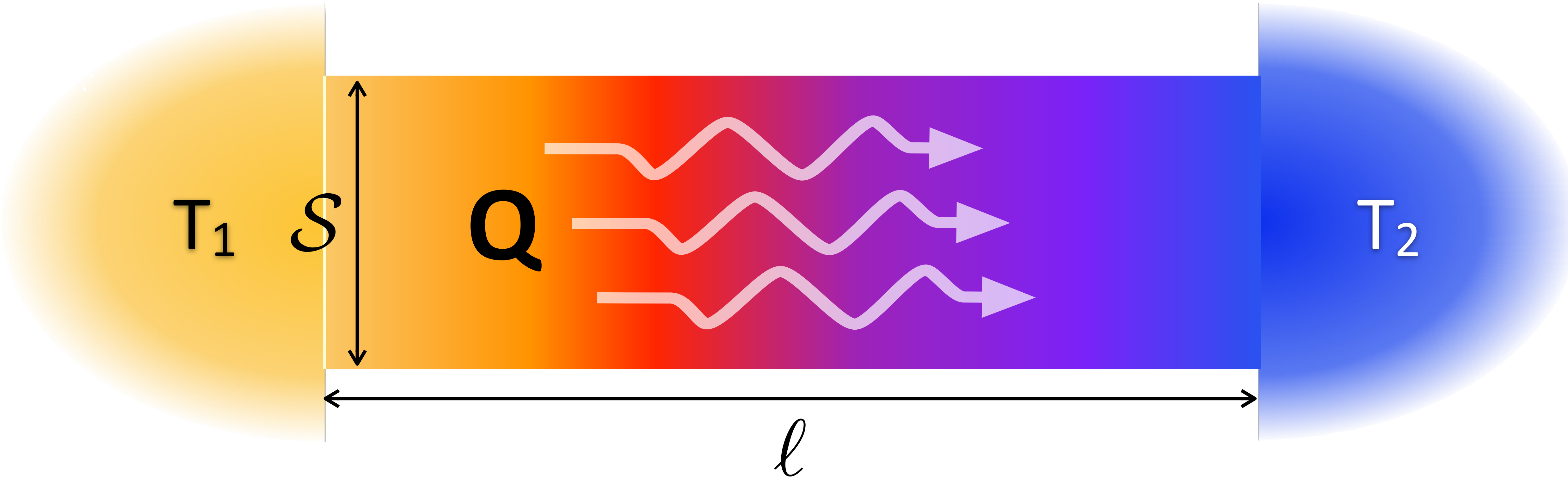
what heat transport is all about



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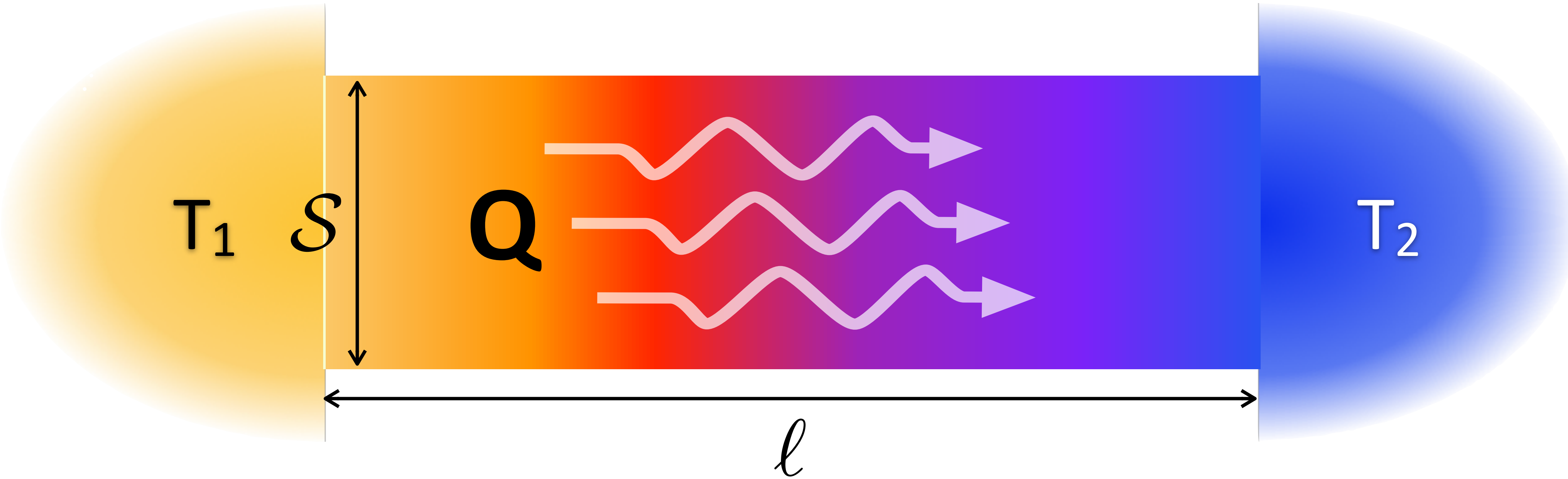
$$\mathbf{j}_Q(\mathbf{r}, t) = -\kappa\nabla T(\mathbf{r}, t)$$

what heat transport is all about



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$$j_Q(\mathbf{r}, t) = -\kappa\nabla T(\mathbf{r}, t)$$

$$\frac{\partial T}{\partial t} = \frac{\kappa}{\rho c_p}\Delta T$$

why should we care?

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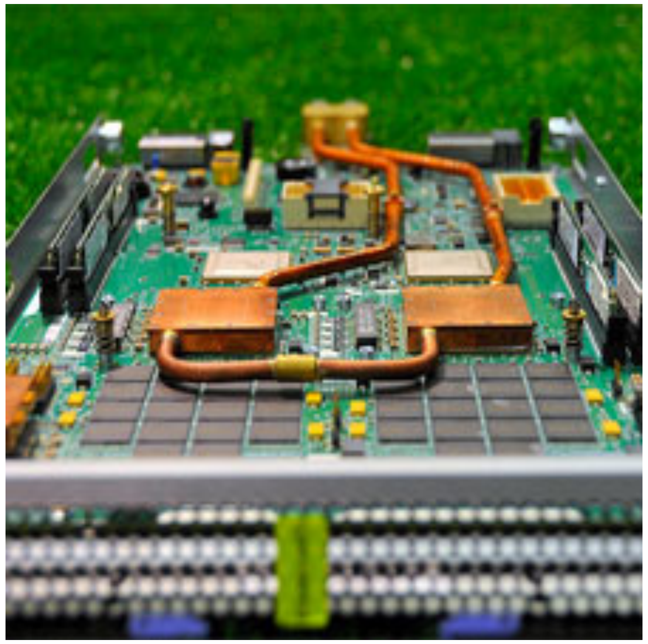
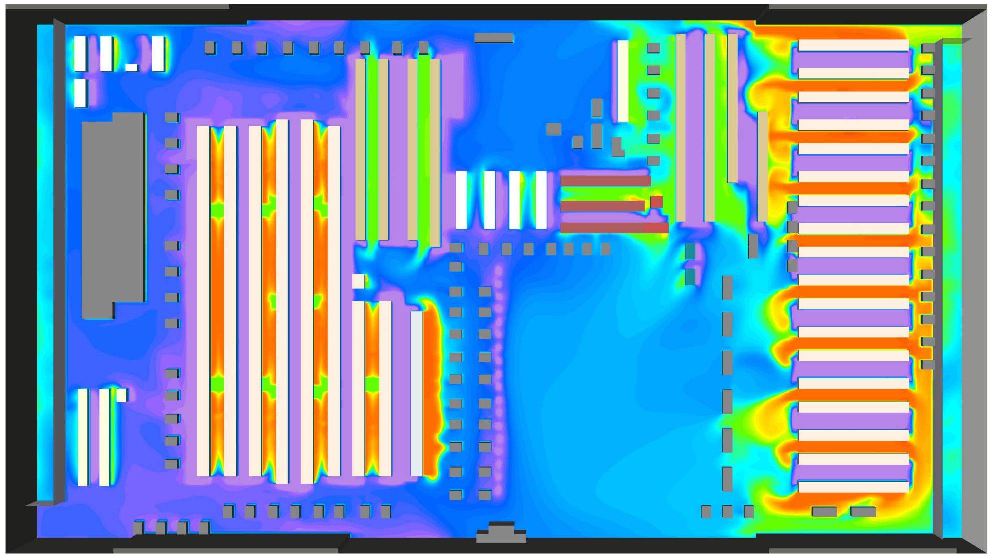
energy saving

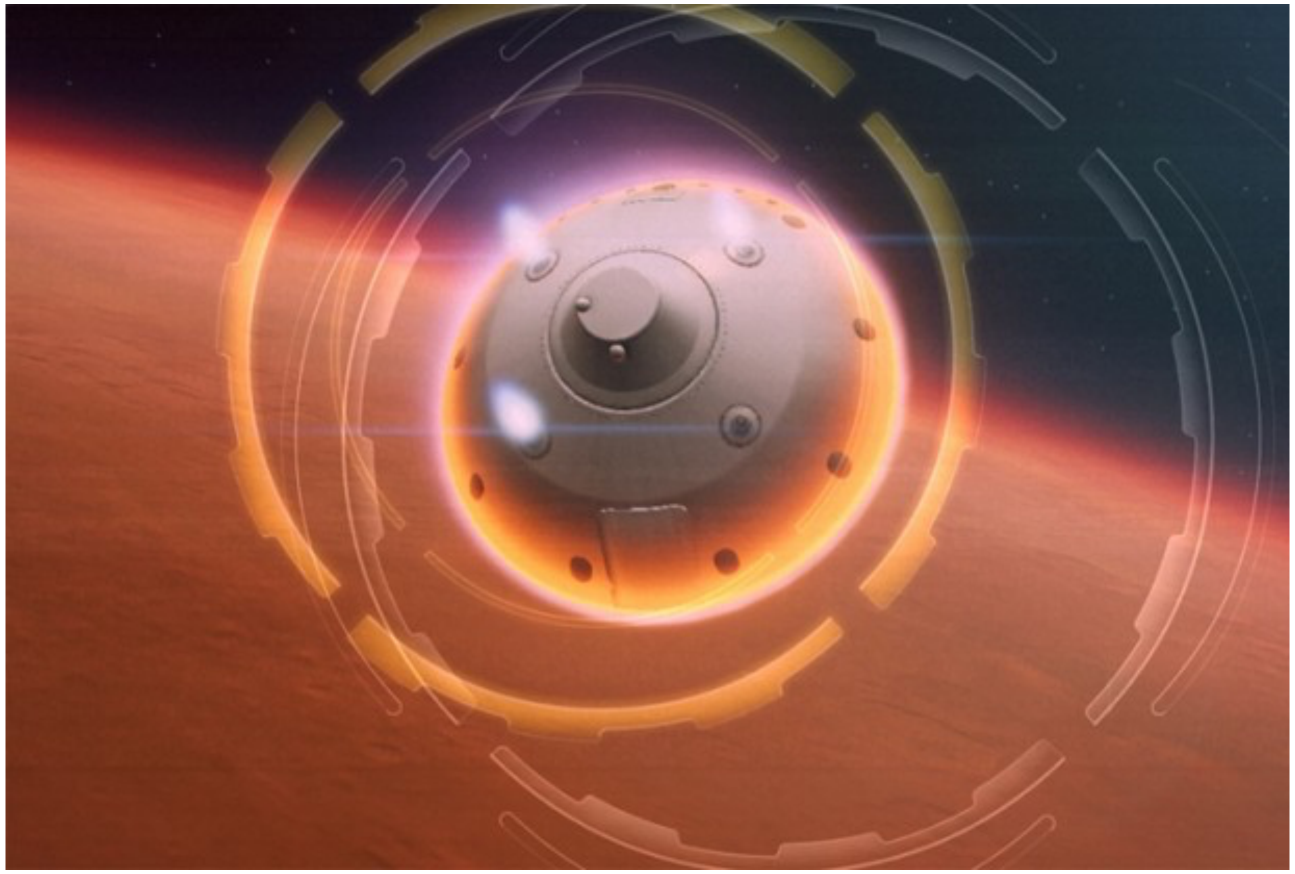
heat dissipation

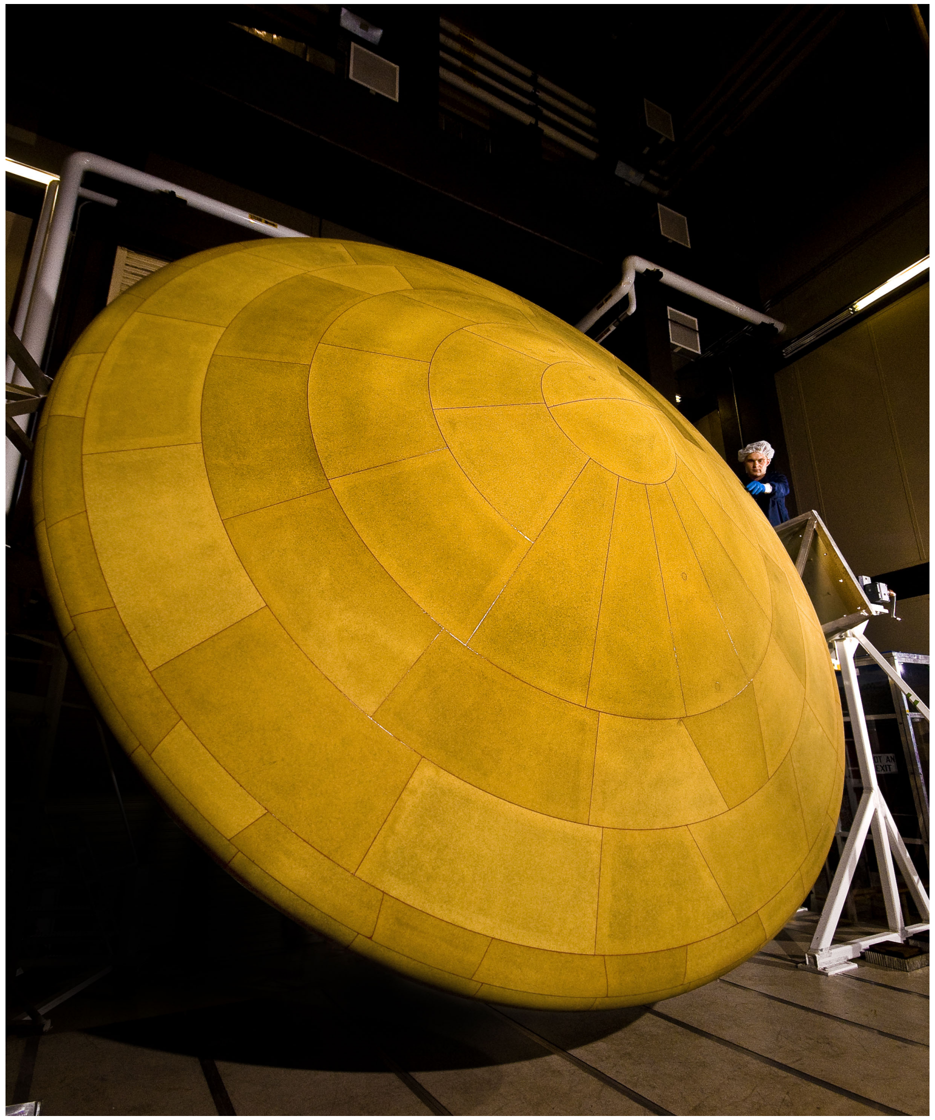




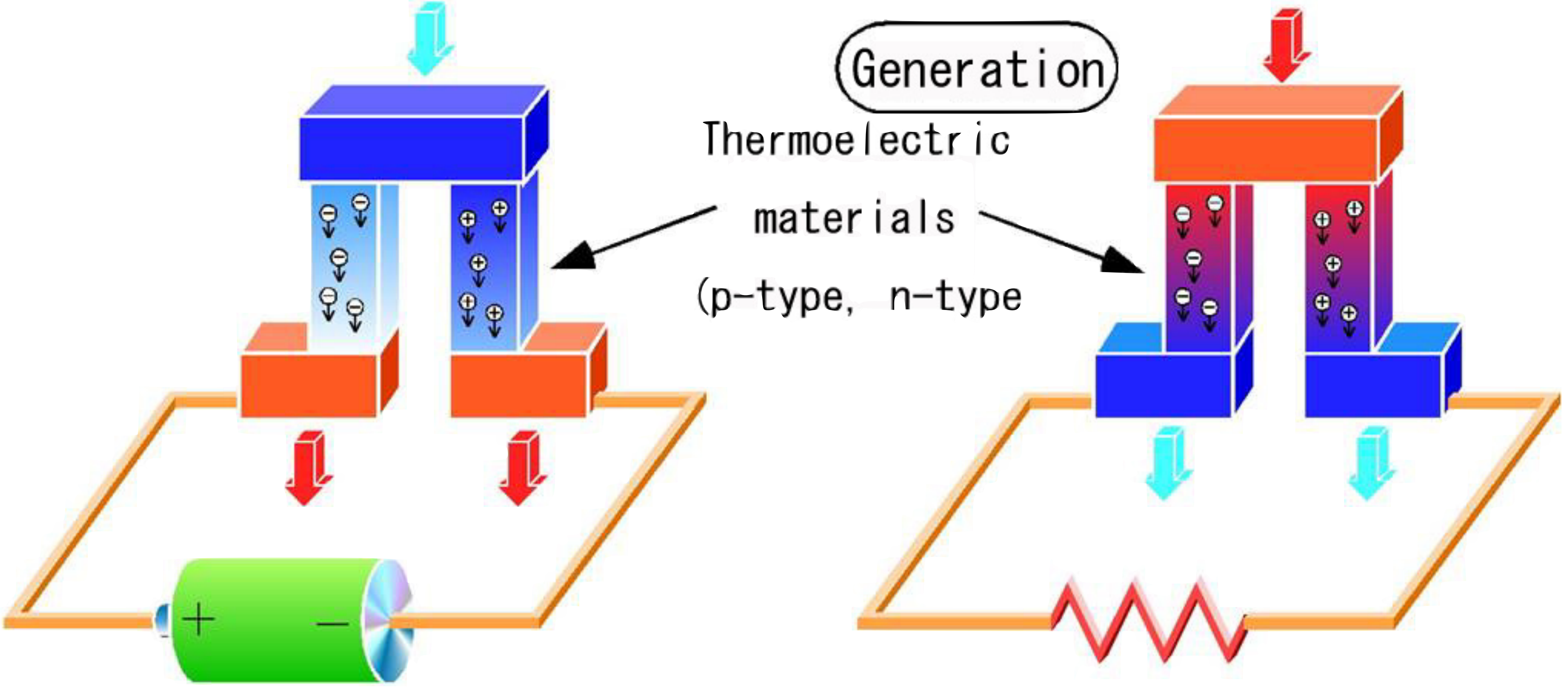
heat shielding

heat shielding

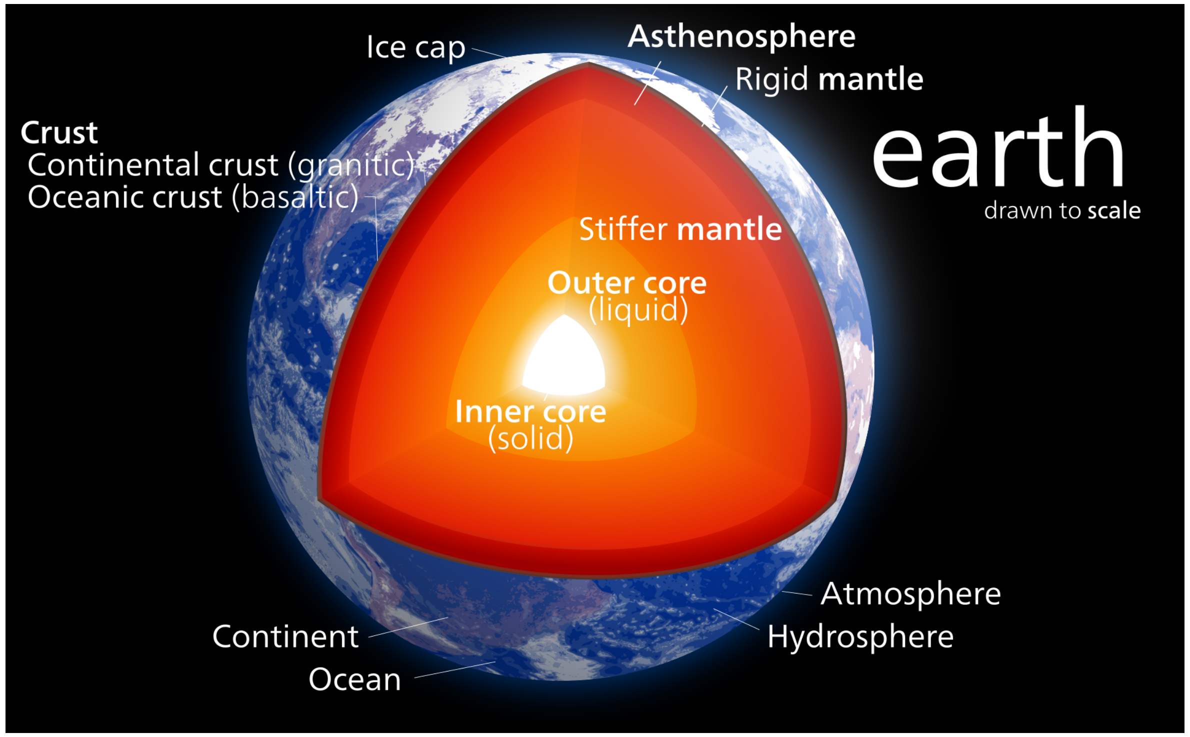


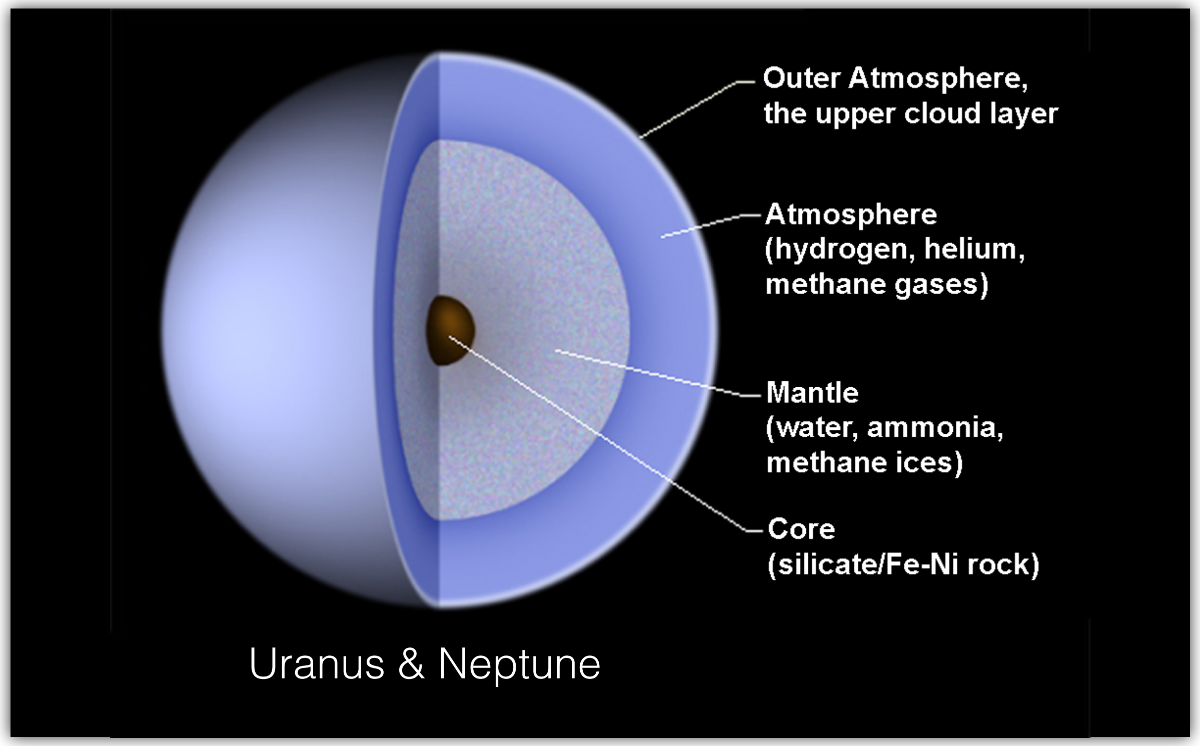


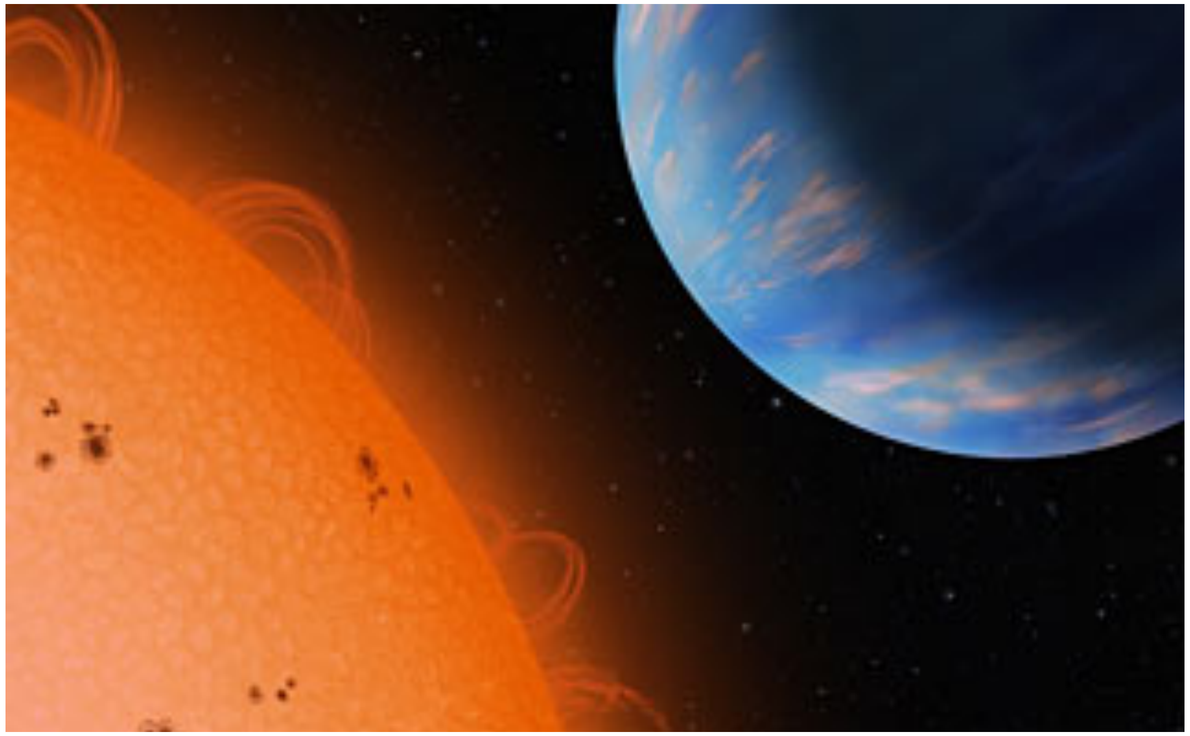
energy conversion

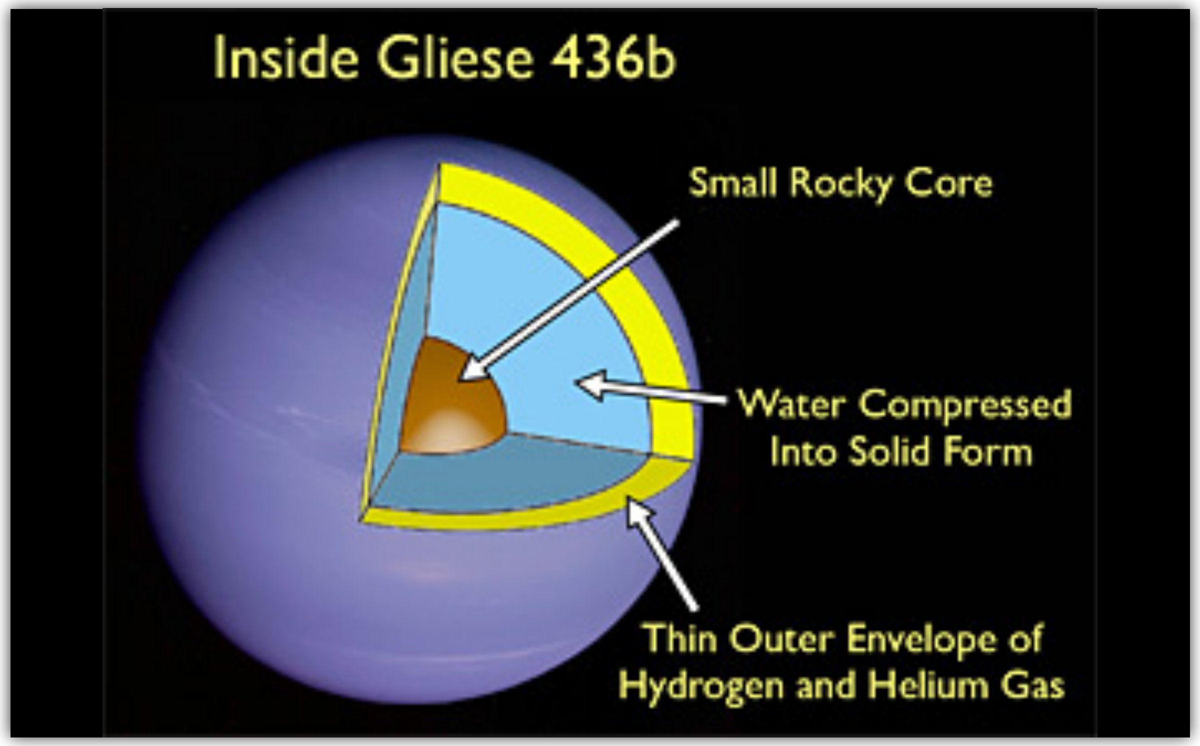


planetary sciences





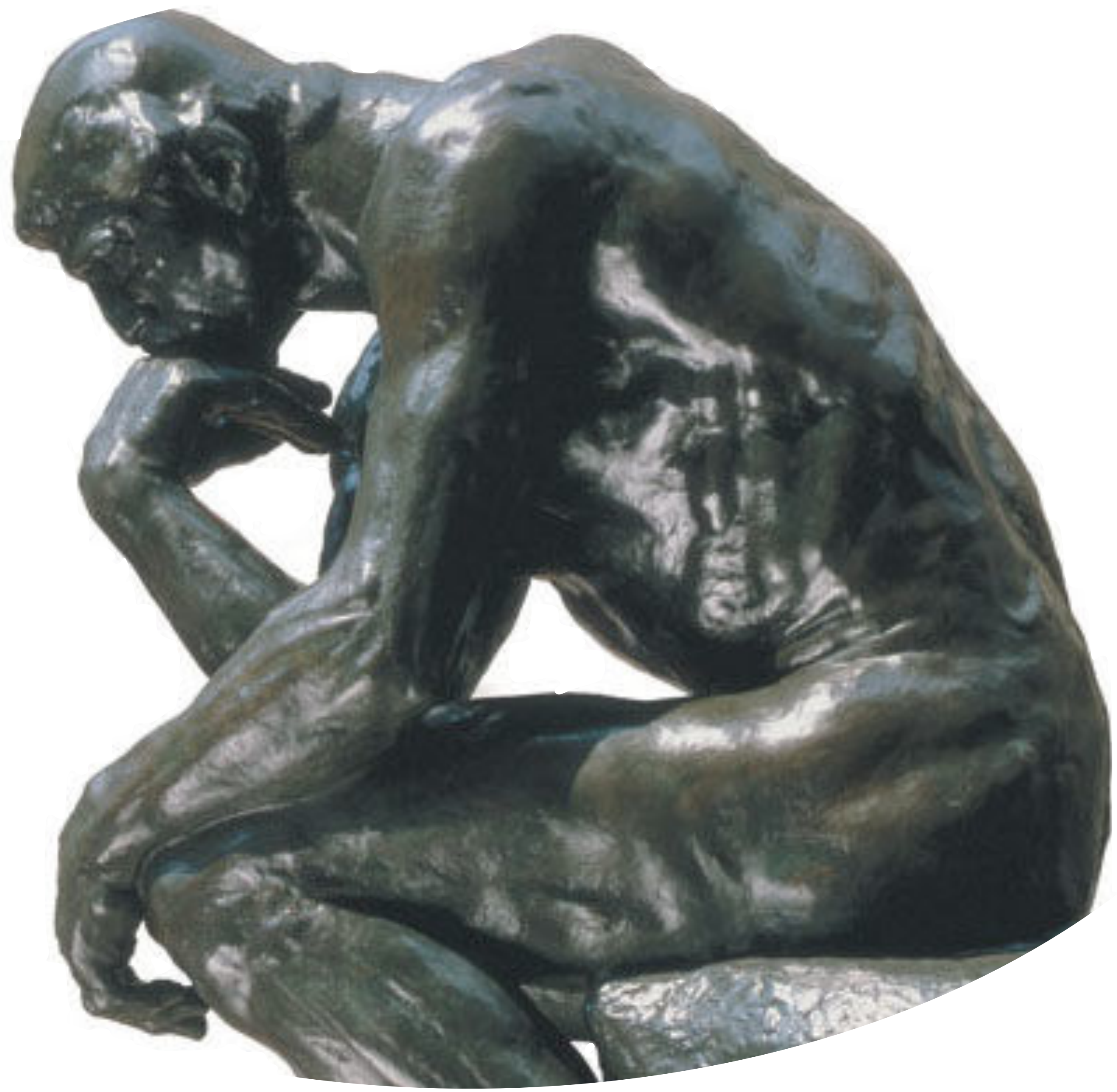




why should we care?

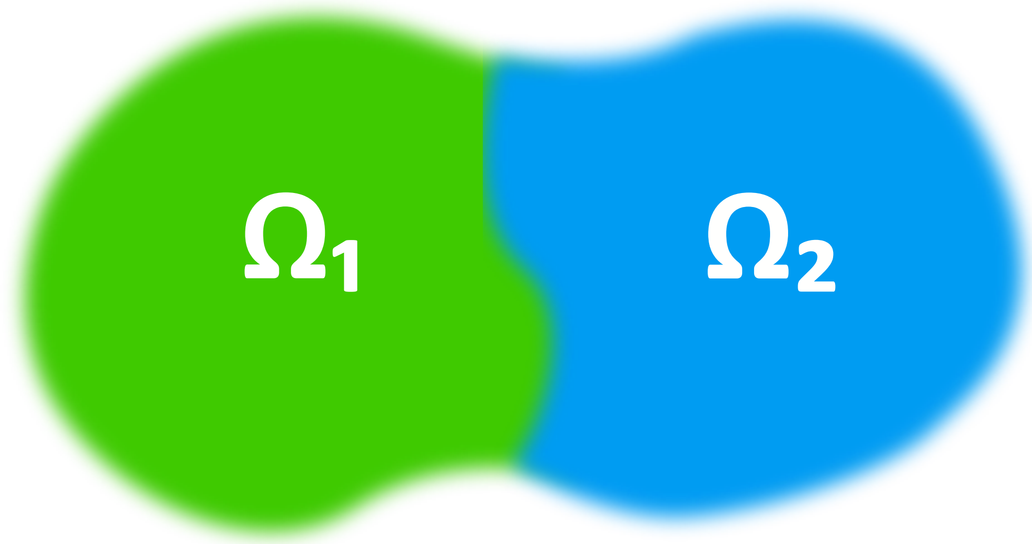
- energy saving and heat dissipation
- heat shielding
- energy conversion
- earth and planetary sciences
- …

why should we care?



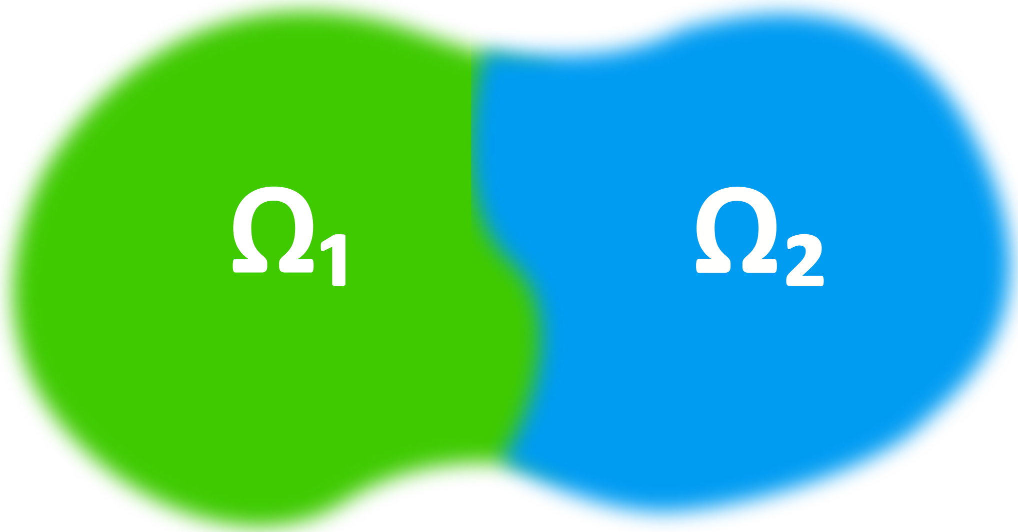
- … because it is important and still poorly understood

extensive properties



$$E[\Omega_1 \cup \Omega_2] = E[\Omega_1] + E[\Omega_2]$$

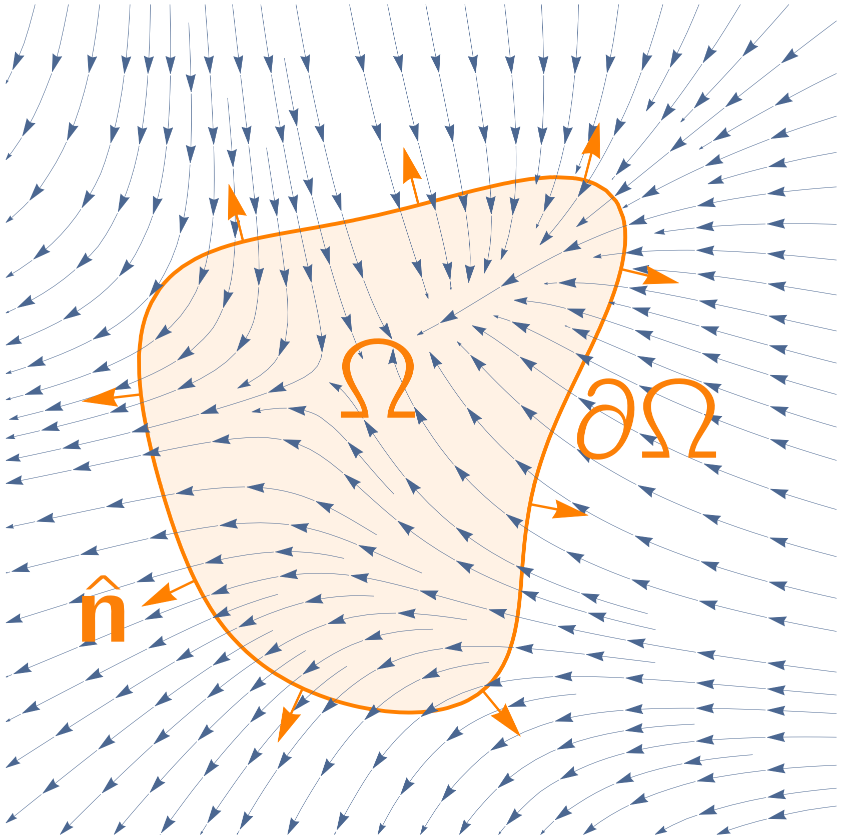
extensive properties



$$E[\Omega_1 \cup \Omega_2] = E[\Omega_1] + E[\Omega_2]$$

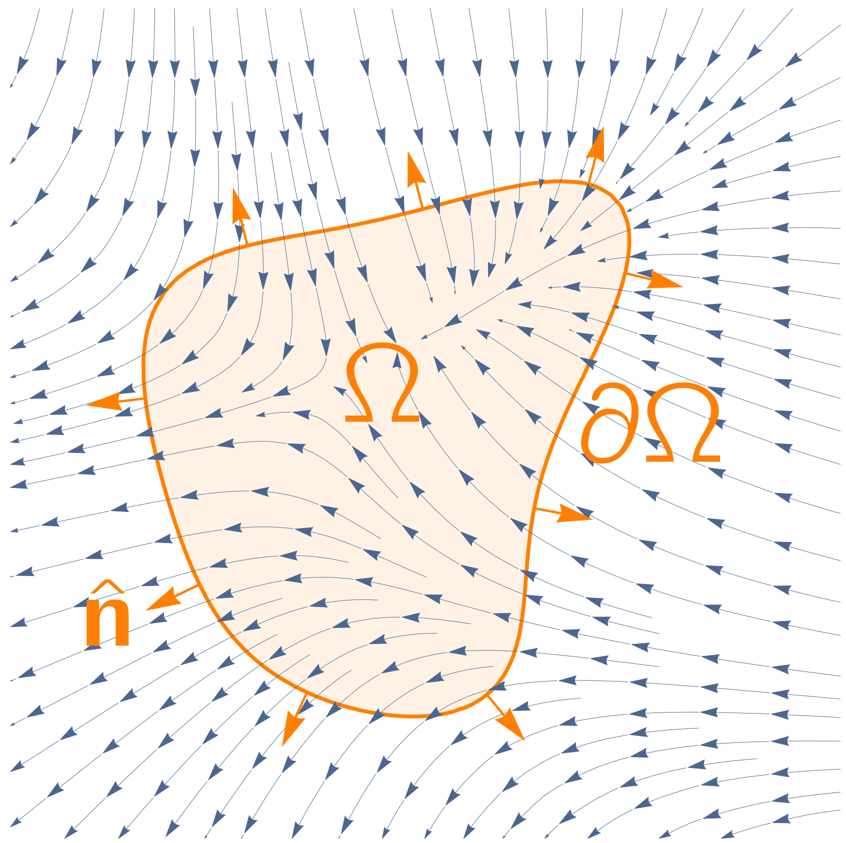
$$E[\Omega] = \int_\Omega \epsilon(\mathbf{r}) d\mathbf{r}$$

conservation laws



$$\frac{dE(\Omega,t)}{dt} = -\oint_{\partial\Omega} \mathbf{j}(\mathbf{r},t)\cdot\hat{\mathbf{n}}\, dS + \int_{\Omega} \sigma(\mathbf{r},t)\, d\Omega$$

conservation laws



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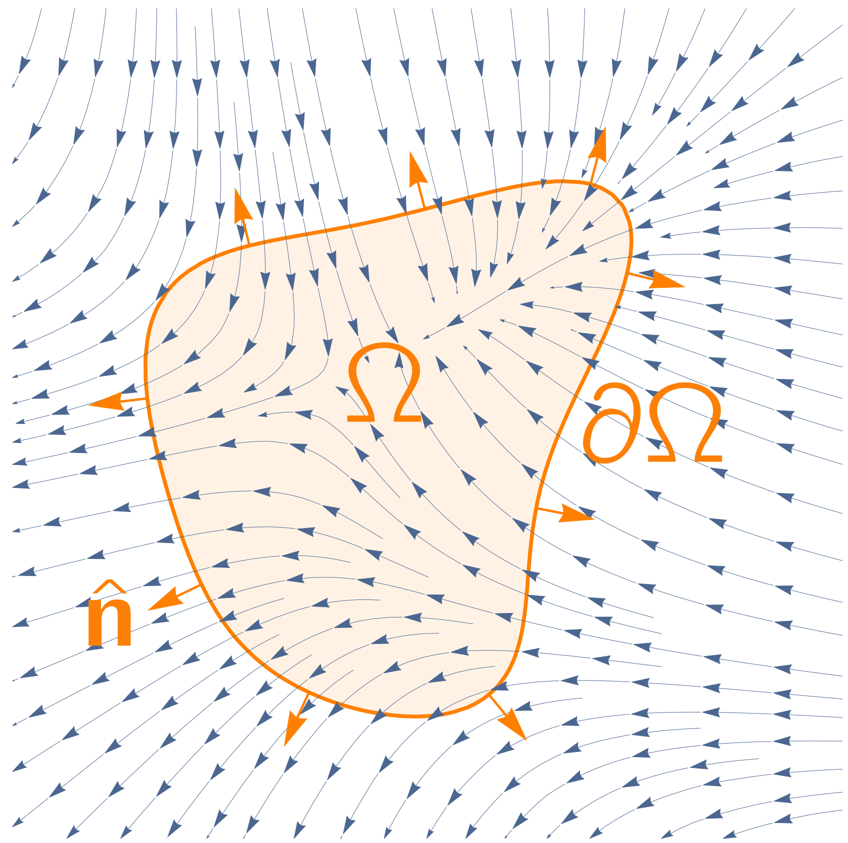

$$\frac{dE(\Omega, t)}{dt} = -\oint_{\partial\Omega} \mathbf{j}(\mathbf{r}, t) \cdot \hat{\mathbf{n}}\, dS + \cancel{\int_{\Omega} \sigma(\mathbf{r}, t) d\Omega}$$

$$\int_{\Omega} \dot{\epsilon}(\mathbf{r}, t) d\Omega = -\int_{\Omega} \nabla \cdot \mathbf{j}(\mathbf{r}, t) d\Omega$$

$$\dot{\epsilon}(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0$$

continuity equation

constitutive relations: Onsager's equations

P conserved quantities: $\left(A_1, A_2, \cdots A_P\right)$

P conserved (current) densities: $\left(a_1(\mathbf{r}), \cdots a_P(\mathbf{r})\right)$, $\left(\mathbf{j}_1(\mathbf{r}), \cdots \mathbf{j}_P(\mathbf{r})\right)$

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At thermodynamic equilibrium: $S = \max$

$$\frac{\delta}{\delta a_i}\Big(S - \sum_j \lambda_j A_j\Big) = 0$$

$$\frac{\delta S}{\delta a_i} = \alpha_i(\mathbf{r}) = \lambda_i$$

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Onsager's linear-response equations

$$\Lambda_{ij} = \Lambda_{ji}$$

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Onsager's linear-response equations

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A	$\alpha = \frac{\partial S}{\partial A}$
E	$\frac{1}{T}$
V	$\frac{p}{T}$
N_i	$-\frac{\mu_i}{T}$

Green-Kubo linear-response theory

$$\Lambda_{ij} = \frac{\Omega}{k_B} \int_0^\infty \langle J_i(t) J_j(0) \rangle dt$$

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Einstein-Helfand relations

Einstein (1905)

$$\left\langle |x(t) - x(0)|^2 \right\rangle = \left\langle \left| \int_0^t v(t')dt' \right|^2 \right\rangle$$

$$\approx 2Dt$$

$$D = \int_0^\infty \langle v(t)v(0)\rangle dt$$

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Helfand (1960)

$$\left\langle \left| \int_0^t J(t')dt' \right|^2 \right\rangle \approx 2\Lambda t$$

$$\Lambda = \int_0^\infty \langle J(t)J(0) \rangle dt$$

the classical energy current

$$\mathbf{J} = \frac{1}{\Omega}\int_\Omega \mathbf{j}(\mathbf{r})d\mathbf{r}$$

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$$\int_\Omega \mathbf{r}\big(\nabla\cdot\mathbf{j}(\mathbf{r})\big)d\mathbf{r} = -\int_\Omega \mathbf{r}\dot{\epsilon}(\mathbf{r})d\mathbf{r}$$

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$$\mathbf{J} = \sum_I \big(\dot{\mathbf{R}}_I e_I + \mathbf{R}_I \dot{e}_I\big)$$

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$$\mathbf{J} = \sum_{I} e_I \mathbf{V}_I + \frac{1}{2}\sum_{I\neq J}(\mathbf{V}_I\cdot\mathbf{F}_{IJ})(\mathbf{R}_I - \mathbf{R}_J)$$

hurdles towards an ab initio Green-Kubo theory

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Thermal Conductivity of Periclase (MgO) from First Principles

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Department of Computer Science, Louisiana State University, Baton Rouge, Louisiana 70803, USA
and Department of Geology and Geophysics, Louisiana State University, Baton Rouge, Louisiana 70803, USA

sensitive to the form of the potential. The widely used Green-Kubo relation [14] does not serve our purposes, because in first-principles calculations it is impossible to uniquely decompose the total energy into individual contributions from each atom.

insights from classical mechanics

$$E = \sum_I \epsilon_I(\mathbf{R}, \mathbf{V})$$

$$= \mathsf{cnst}$$

$$\epsilon_I(\mathbf{R}, \mathbf{V}) = \frac{1}{2} M_I \mathsf{V}_I^2 + \frac{1}{2} \sum_{J \neq I} v(|\mathbf{R}_I - \mathbf{R}_J|)$$

$$\mathbf{J}_e = \sum_I \epsilon_I \mathbf{V}_I + \frac{1}{2} \sum_{I \neq J} (\mathbf{V}_I \cdot \mathbf{F}_{IJ})(\mathbf{R}_I - \mathbf{R}_J)$$

insights from classical mechanics

$$\sum_I \epsilon_I(\mathbf{R},\mathbf{V}) = \mathrm{cnst}$$

$$\epsilon_I(\mathbf{R},\mathbf{V}) = \frac{1}{2} M_I \mathsf{V}_I^2 + \frac{1}{2}\sum_{J\neq I} v(|\mathbf{R}_I - \mathbf{R}_J|)(1+\Gamma_{IJ})$$

$$\mathbf{J}_e = \sum_I \epsilon_I \mathbf{V}_I + \frac{1}{2}\sum_{I\neq J}(\mathbf{V}_I\cdot\mathbf{F}_{IJ})(\mathbf{R}_I-\mathbf{R}_J)$$

$$+\frac{1}{2}\sum_{I\neq J}\Gamma_{IJ}\left[\mathbf{V}_I v(|\mathbf{R}_I-\mathbf{R}_J|) + (\mathbf{V}_I\cdot\mathbf{F}_{IJ})(\mathbf{R}_I-\mathbf{R}_I)\right]$$

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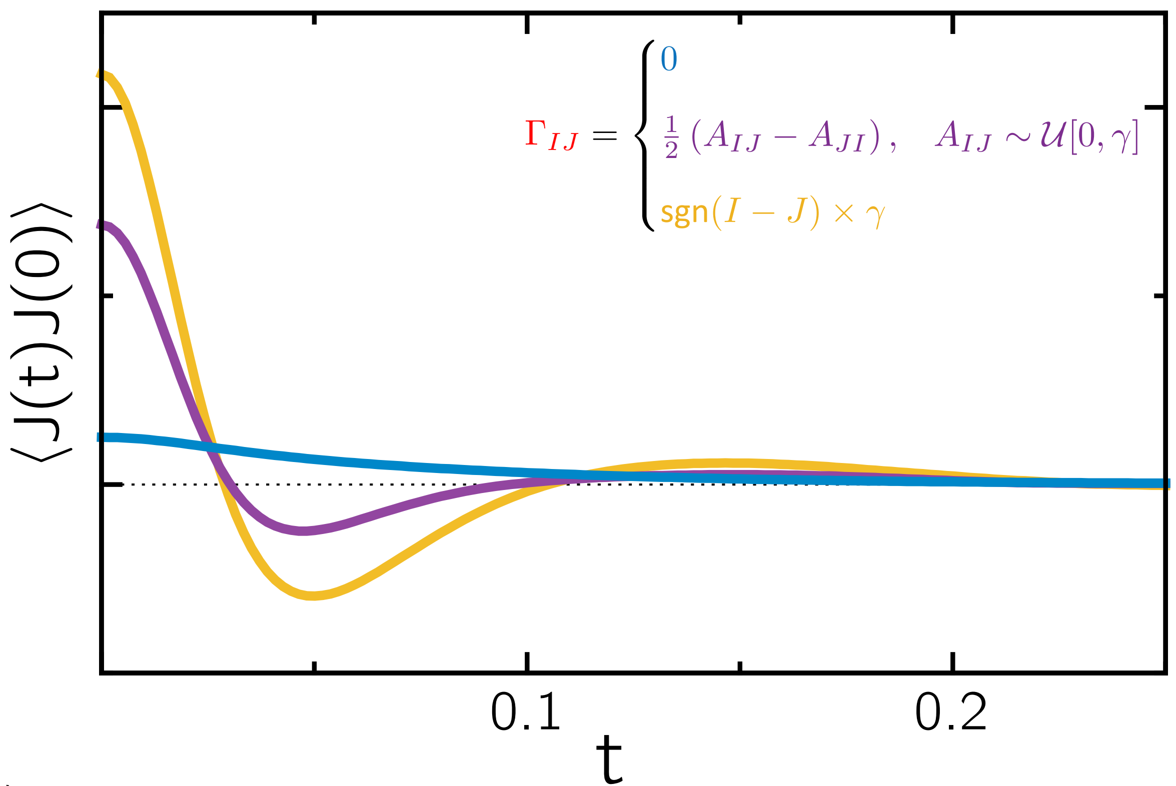

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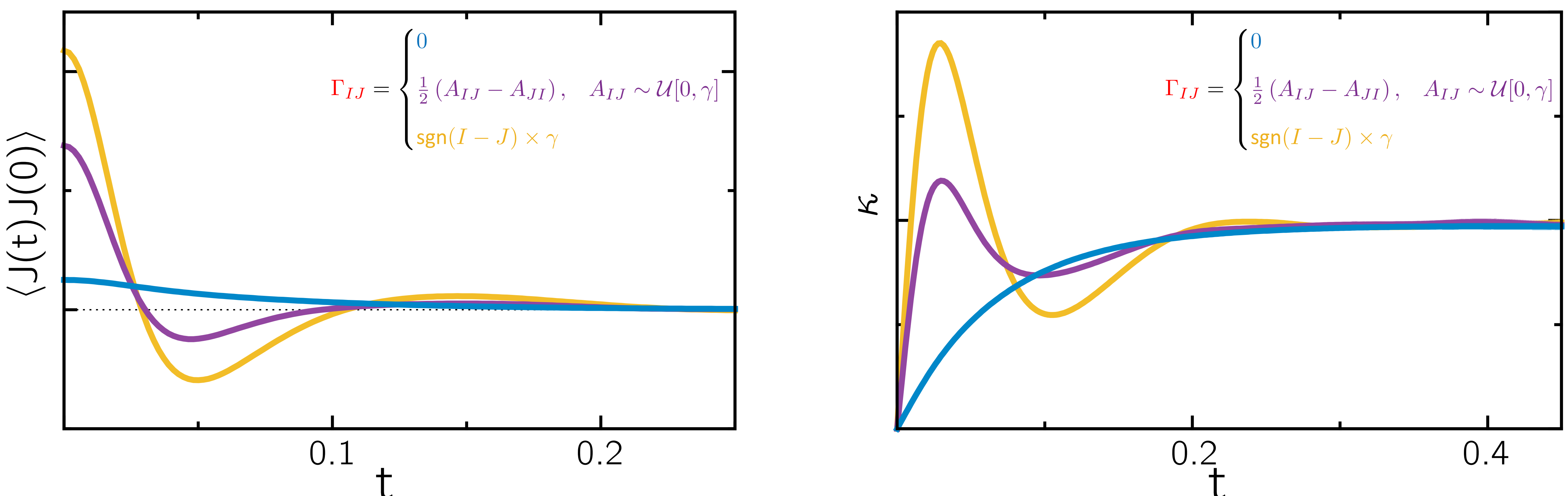

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insights from classical mechanics

$$\mathbf{J}_e = \sum_I \epsilon_I \mathbf{V}_I + \frac{1}{2}\sum_{I\neq J}(\mathbf{V}_I \cdot \mathbf{F}_{IJ})(\mathbf{R}_I - \mathbf{R}_J)$$
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$$\dot{\mathbf{P}} = \frac{\mathrm{d}}{\mathrm{dt}}\frac{1}{4}\sum_{I\neq J}\Gamma_{IJ}\, v(|\mathbf{R}_I - \mathbf{R}_J|)(\mathbf{R}_I - \mathbf{R}_I)$$

insights from classical mechanics

$$\mathbf{J}' = \mathbf{J} + \dot{\mathbf{P}}$$

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insights from classical mechanics

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$$\mathrm{var}\left[\mathbf{D}'(t)\right] = \mathrm{var}\left[\mathbf{D}(t)\right] + \mathrm{var}\left[\Delta\mathbf{P}(t)\right] + 2\mathrm{cov}\left[\mathbf{D}(t)\cdot\Delta\mathbf{P}(t)\right]$$

insights from classical mechanics

$$\mathbf{J}' = \mathbf{J} + \dot{\mathbf{P}}$$

$$\kappa \sim \frac{1}{2t}\mathrm{var}\left[\mathbf{D}(t)\right] \qquad \mathbf{D}(t) = \int_0^t \mathbf{J}(t')dt'$$

$$\mathbf{D}'(t) = \mathbf{D}(t) + \mathbf{P}(t) - \mathbf{P}(0)$$

$$\mathrm{var}\left[\mathbf{D}'(t)\right] = \underbrace{\mathrm{var}\left[\mathbf{D}(t)\right]}_{\mathcal{O}(t)} + \underbrace{\cancel{\mathrm{var}\left[\Delta\mathbf{P}(t)\right]}}_{\mathcal{O}(1)} + \underbrace{\cancel{2\mathrm{cov}\left[\mathbf{D}(t)\cdot\Delta\mathbf{P}(t)\right]}}_{\mathcal{O}(t^{\frac{1}{2}})}$$

insights from classical mechanics

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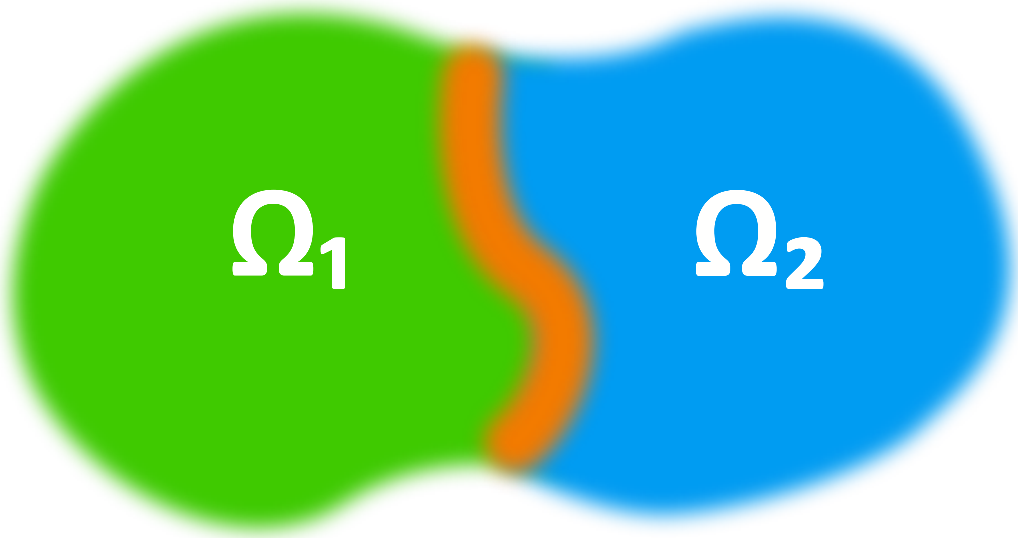
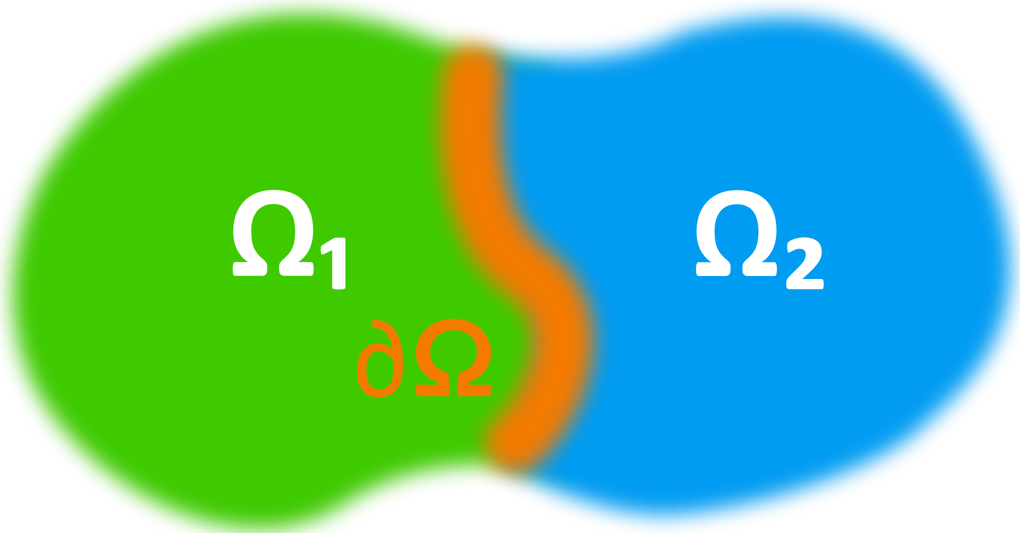
gauge invariance



$$E[\Omega_1 \cup \Omega_2] = E[\Omega_1] + E[\Omega_2] + W[\partial\Omega]$$

gauge invariance



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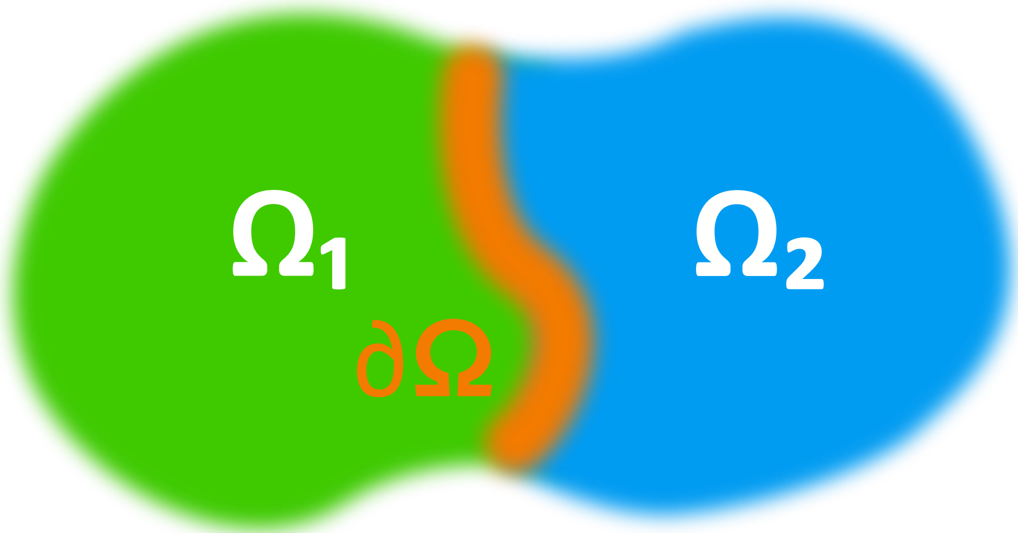

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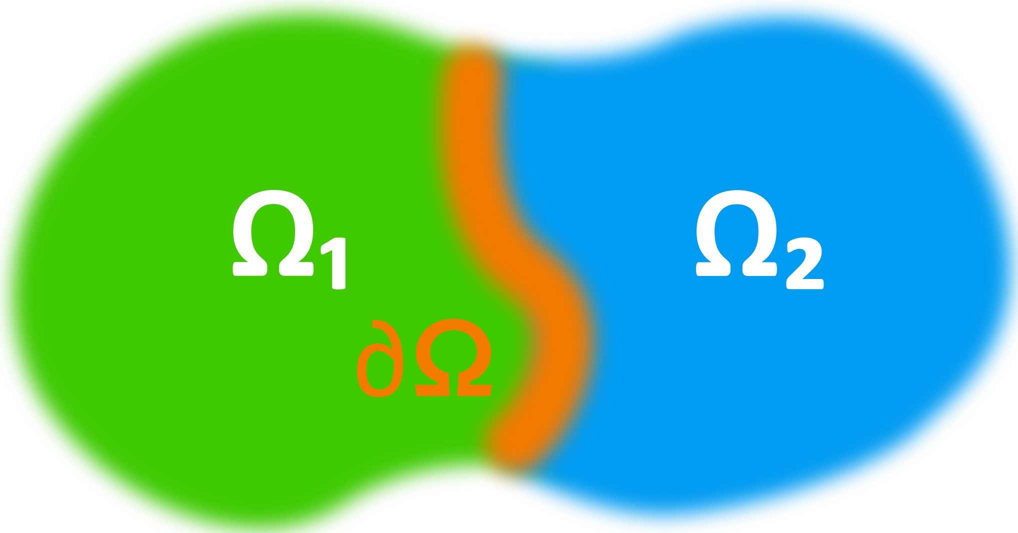

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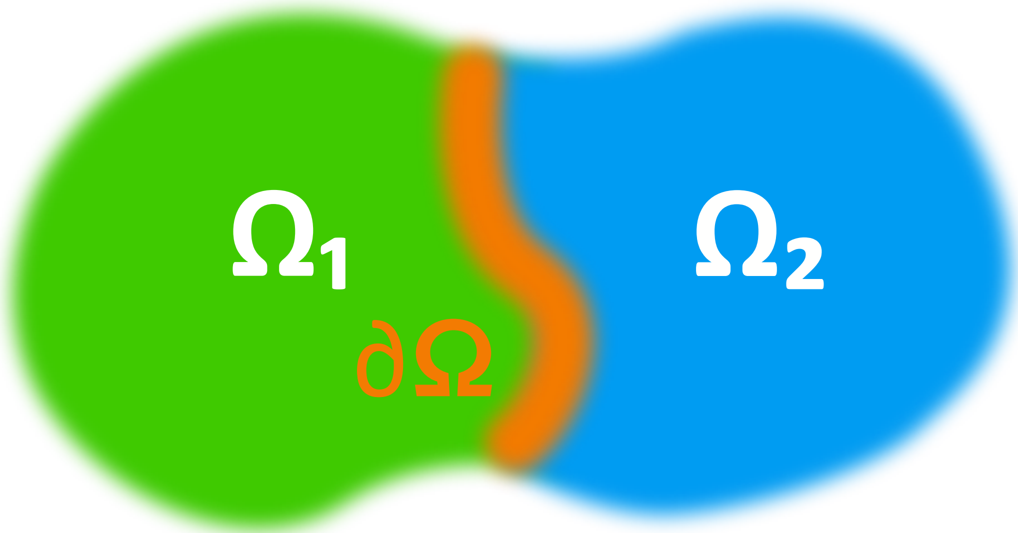

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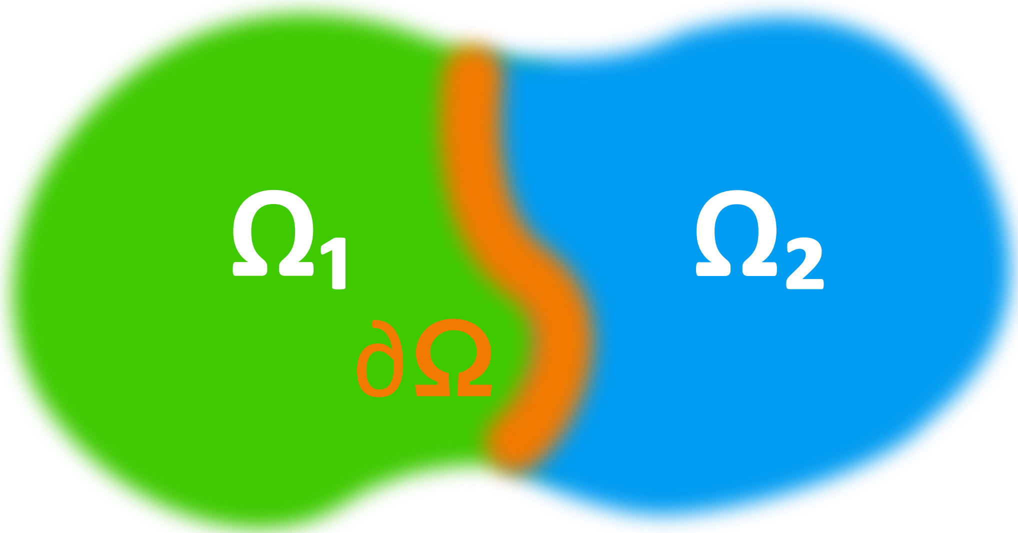

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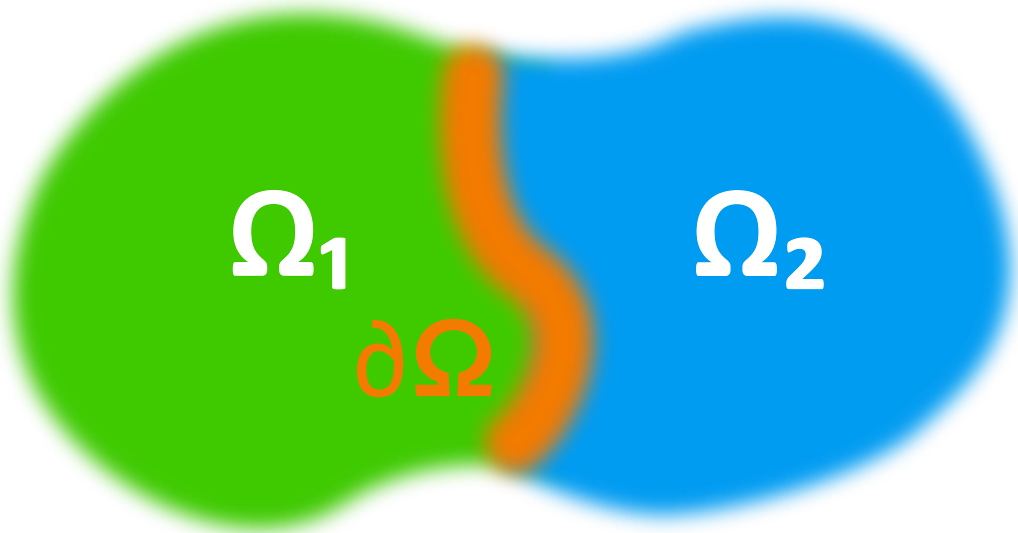

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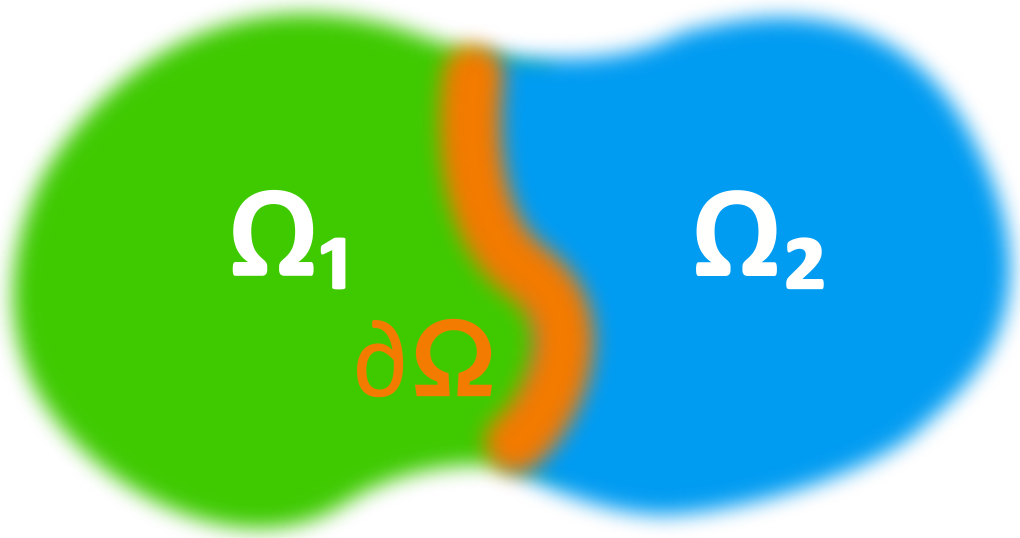

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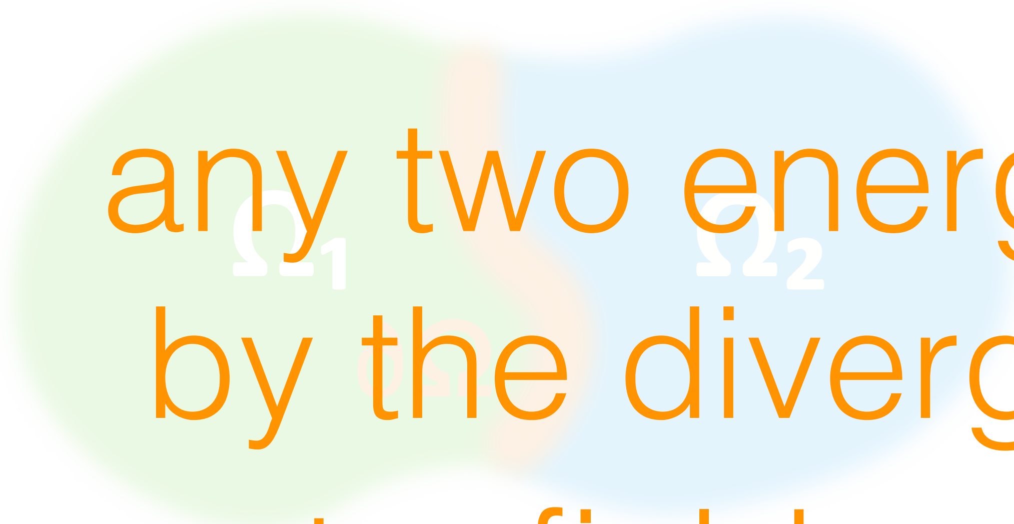

any two energy densities that differ by the divergence of a (bounded) vector field are physically equivalent

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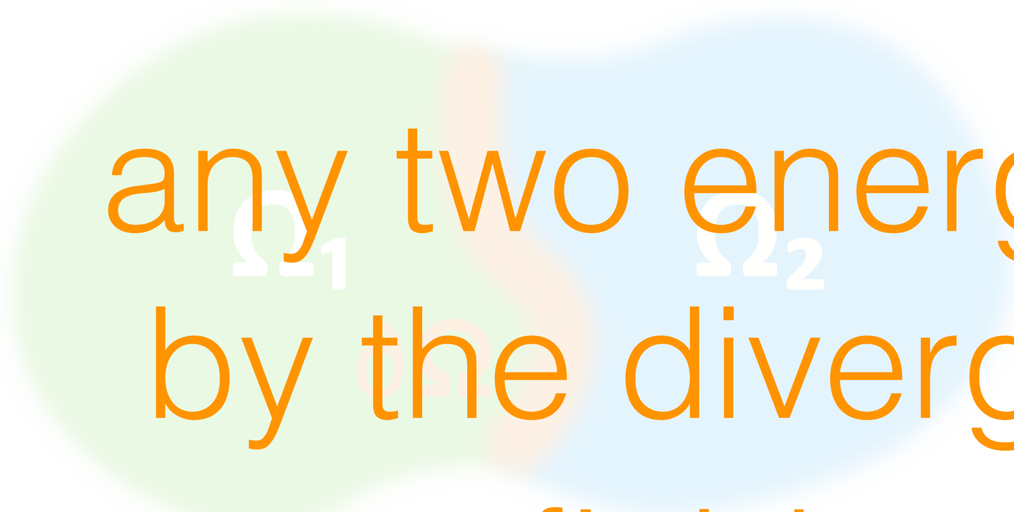

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$$e'(\mathbf{r}) = e(\mathbf{r}) - \nabla \cdot \mathbf{p}(\mathbf{r})$$

the corresponding energy fluxes differ by a total time derivative and the heat transport coefficients coincide

$$\mathbf{j}'(\mathbf{r},t) = \mathbf{j}(\mathbf{r},t) + \dot{\mathbf{p}}(\mathbf{r},t)$$

$$\mathbf{J}'(t) = \mathbf{J}(t) + \dot{\mathbf{P}}(t)$$

density-functional theory

$$
\mathsf{E}_{DFT} = \frac{1}{2}\sum_I M_I \mathsf{V}_I^2 + \frac{\mathsf{e}^2}{2}\sum_{I\neq J}\frac{\mathsf{Z}_I\mathsf{Z}_J}{\mathsf{R}_{IJ}}
$$

$$
+ \sum_v \epsilon_v - \frac{1}{2}\mathsf{E}_H + \int \big(\epsilon_{XC}(\mathbf{r}) - \mu_{XC}(\mathbf{r})\big)\rho(\mathbf{r})d\mathbf{r}
$$

the DFT energy density

$$\mathsf{E}_{DFT} = \frac{1}{2}\sum_I M_I \mathsf{V}_I^2 + \frac{\mathsf{e}^2}{2}\sum_{I\neq J}\frac{\mathsf{Z}_I \mathsf{Z}_J}{\mathsf{R}_{IJ}}$$

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$$e_{DFT}(\mathbf{r}) = e_0(\mathbf{r}) + e_{KS}(\mathbf{r}) + e_H(\mathbf{r}) + e_{XC}(\mathbf{r})$$

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$$e_{DFT}(\mathbf{r}) = e_0(\mathbf{r}) + e_{KS}(\mathbf{r}) + e_H(\mathbf{r}) + e_{XC}(\mathbf{r})$$

$$e_0(\mathbf{r}) = \sum_I \delta(\mathbf{r} - \mathbf{R}_I)\left(\frac{1}{2}M_I V_I^2 + w_I\right)$$

$$e_{KS}(\mathbf{r}) = \mathrm{Re}\sum_v \varphi_v^*(\mathbf{r})\big(\hat{H}_{KS}\varphi_v(\mathbf{r})\big)$$

$$e_H(\mathbf{r}) = -\frac{1}{2}\rho(\mathbf{r})v_H(\mathbf{r})$$

$$e_{XC}(\mathbf{r}) = \big(\epsilon_{XC}(\mathbf{r}) - v_{XC}(\mathbf{r})\big)\,\rho(\mathbf{r})$$

the DFT energy current

$$\mathbf{J}_{DFT} = \int \mathbf{r}\dot{e}_{DFT}(\mathbf{r},t)d\mathbf{r}$$

$$= \mathbf{J}_{KS} + \mathbf{J}_{H} + \mathbf{J}_0' + \mathbf{J}_0 + \mathbf{J}_{XC}$$

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$$\mathbf{J}_{KS} = \sum_v \Big(\langle \varphi_v | \mathbf{r} \hat{H}_{KS} | \dot{\varphi}_v \rangle + \varepsilon_v \langle \dot{\varphi}_v | \mathbf{r} | \varphi_v \rangle \Big)$$

$$\mathbf{J}_H = \frac{1}{4\pi} \int \dot{v}_H(\mathbf{r}) \nabla v_H(\mathbf{r}) d\mathbf{r}$$

$$\mathbf{J}_0' = \sum_{v,I} \langle \varphi_v | (\mathbf{r} - \mathbf{R}_I) (\mathbf{V}_I \cdot \nabla_I \hat{v}_0) | \varphi_v \rangle$$

$$\mathbf{J}_0 = \sum_I \Big[\mathbf{V}_I e_I^0 + \sum_{L \neq I} (\mathbf{R}_I - \mathbf{R}_L) (\mathbf{V}_L \cdot \nabla_L w_I) \Big]$$

$$\mathbf{J}_{XC} = \begin{cases} 0 & \text{(LDA)} \\ -\int \rho(\mathbf{r}) \dot{\rho}(\mathbf{r}) \partial \epsilon_{GGA}(\mathbf{r}) d\mathbf{r} & \text{(GGA)} \end{cases}$$

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$$\mathbf{J}_{DFT} = \int \mathbf{r}\dot{e}_{DFT}(\mathbf{r}, t)d\mathbf{r}$$

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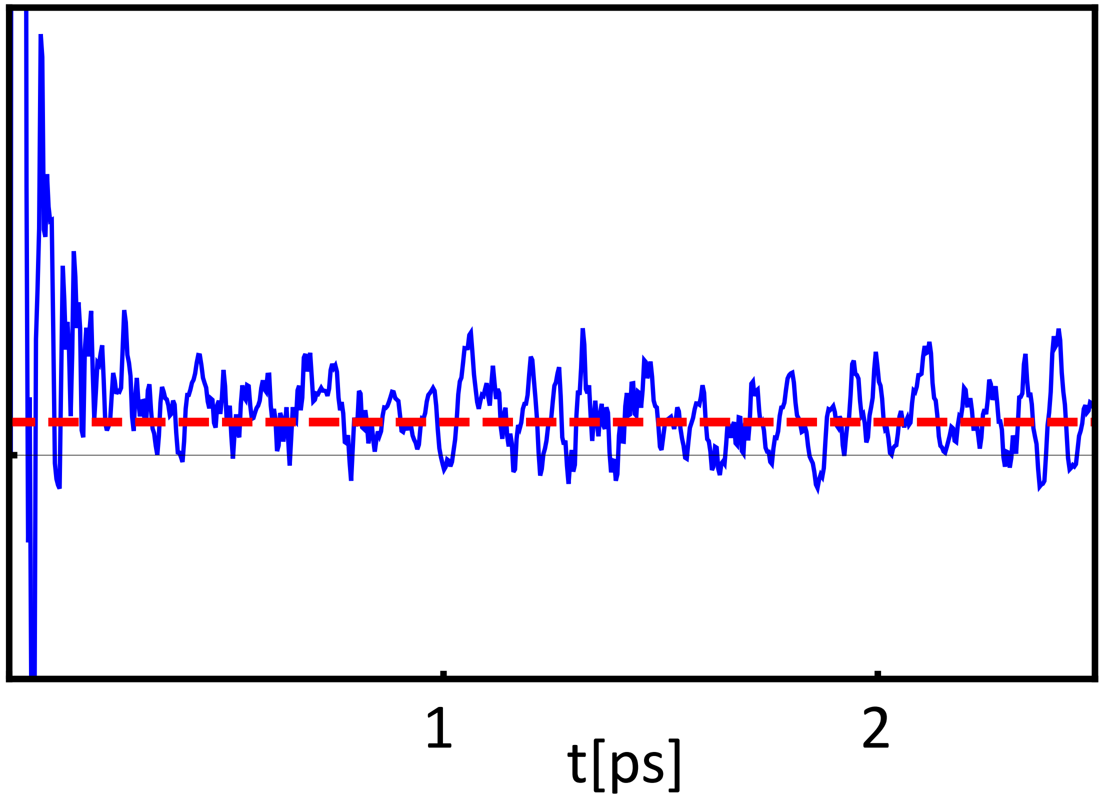
$$\mathbf{J}_H = \frac{1}{4\pi} \int \dot{v}_H(\mathbf{r}) \nabla v_H(\mathbf{r}) d\mathbf{r}$$

- $|\dot{\varphi}_v\rangle$ and $\hat{H}_{KS}|\dot{\varphi}_v\rangle$ orthogonal to the occupied-state manifold
- $\hat{P}_c \mathbf{r} |\varphi_v\rangle$ computed from standard DFPT

$$\mathbf{J}_{XC} = \begin{cases} 0 & \text{(LDA)} \\ -\int \rho(\mathbf{r}) \dot{\rho}(\mathbf{r}) \partial \epsilon_{GGA}(\mathbf{r}) d\mathbf{r} & \text{(GGA)} \end{cases}$$

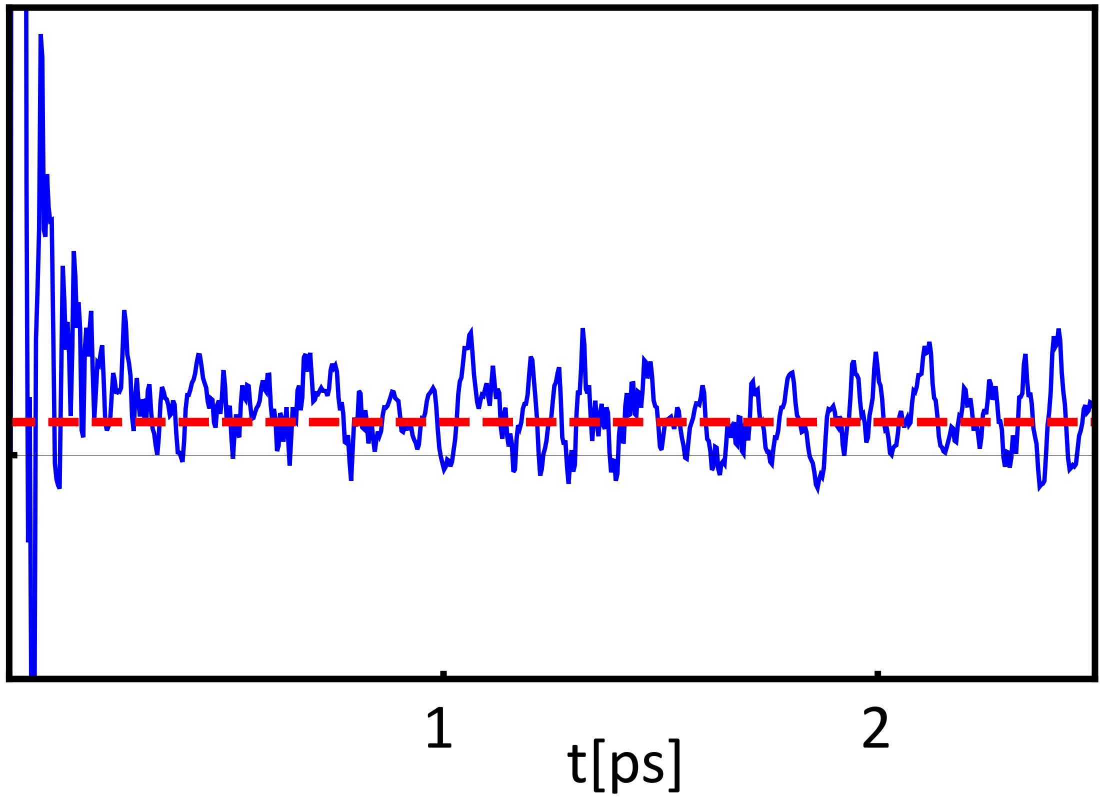
liquid (heavy) water



64 molecules, T=385 K
expt density @ac

$$\frac{1}{3Vk_BT^2}\int_0^{t}\langle \mathbf{J}(t')\cdot\mathbf{J}(0)\rangle dt'$$

liquid (heavy) water



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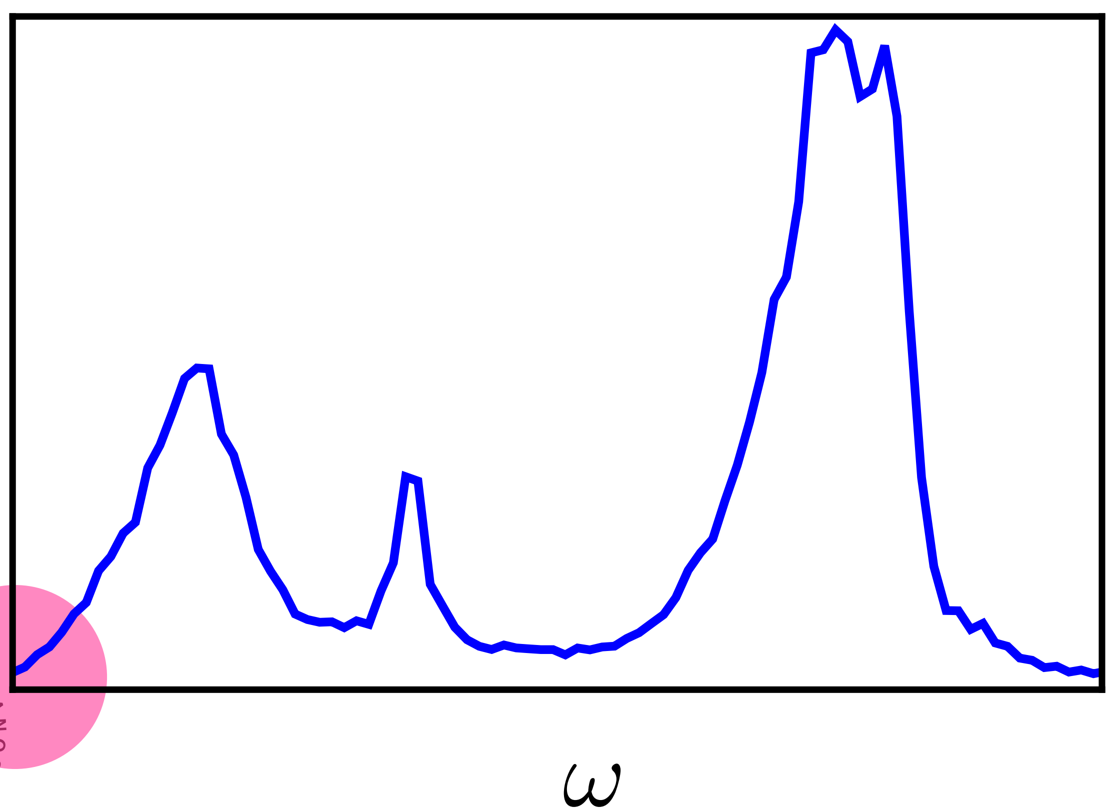
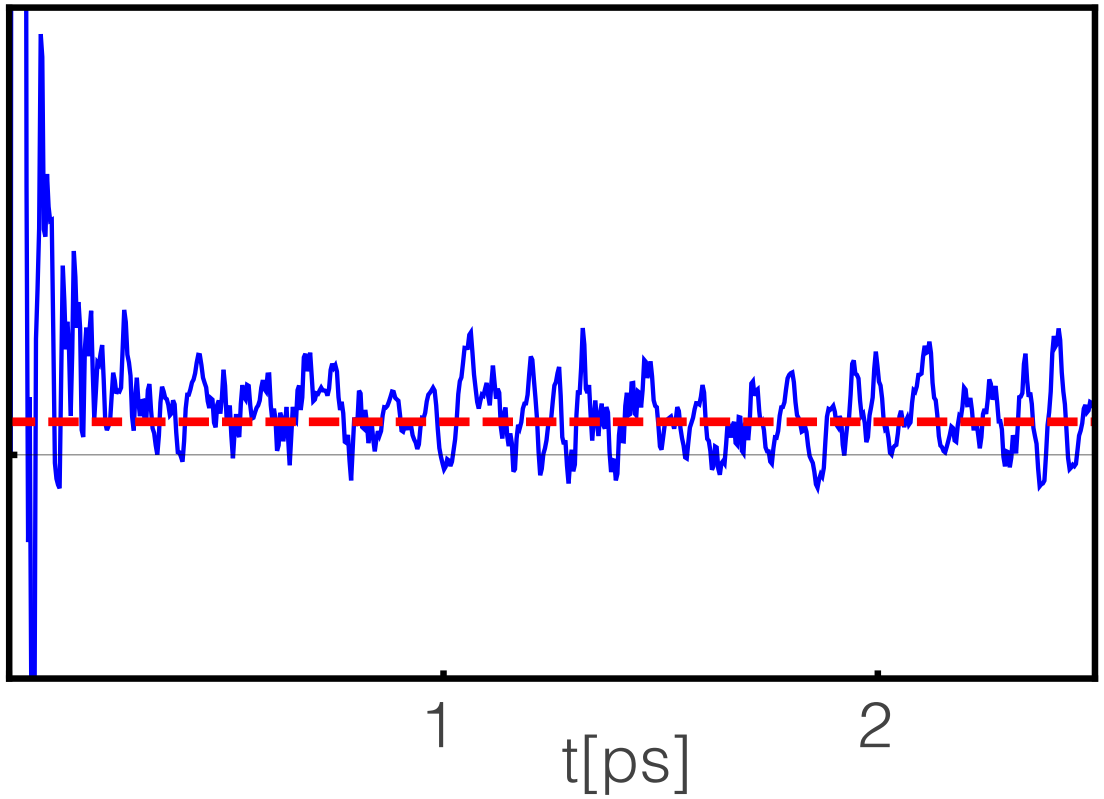
$$\frac{1}{3Vk_BT^2}\int_0^{\mathsf{t}}\langle\mathbf{J}(\mathsf{t}')\cdot\mathbf{J}(0)\rangle d\mathsf{t}'$$



$$S(\omega)=\int_{-\infty}^{\infty}\langle\mathbf{J}(\mathsf{t})\cdot\mathbf{J}(0)\rangle\,\mathsf{e}^{i\omega\mathsf{t}}d\mathsf{t}$$

liquid (heavy) water



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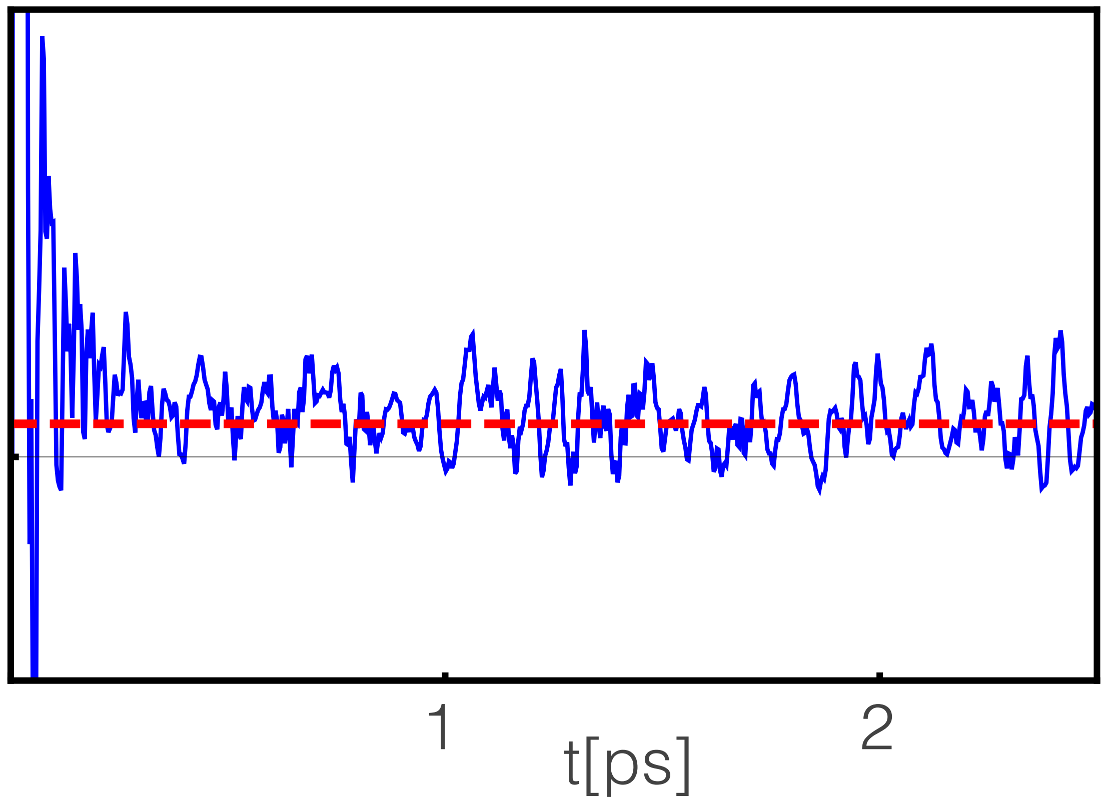
$$\frac{1}{3Vk_BT^2}\int_0^{\mathsf{t}}\langle \mathbf{J}(\mathsf{t}')\cdot\mathbf{J}(0)\rangle d\mathsf{t}'$$

Einstein's relation

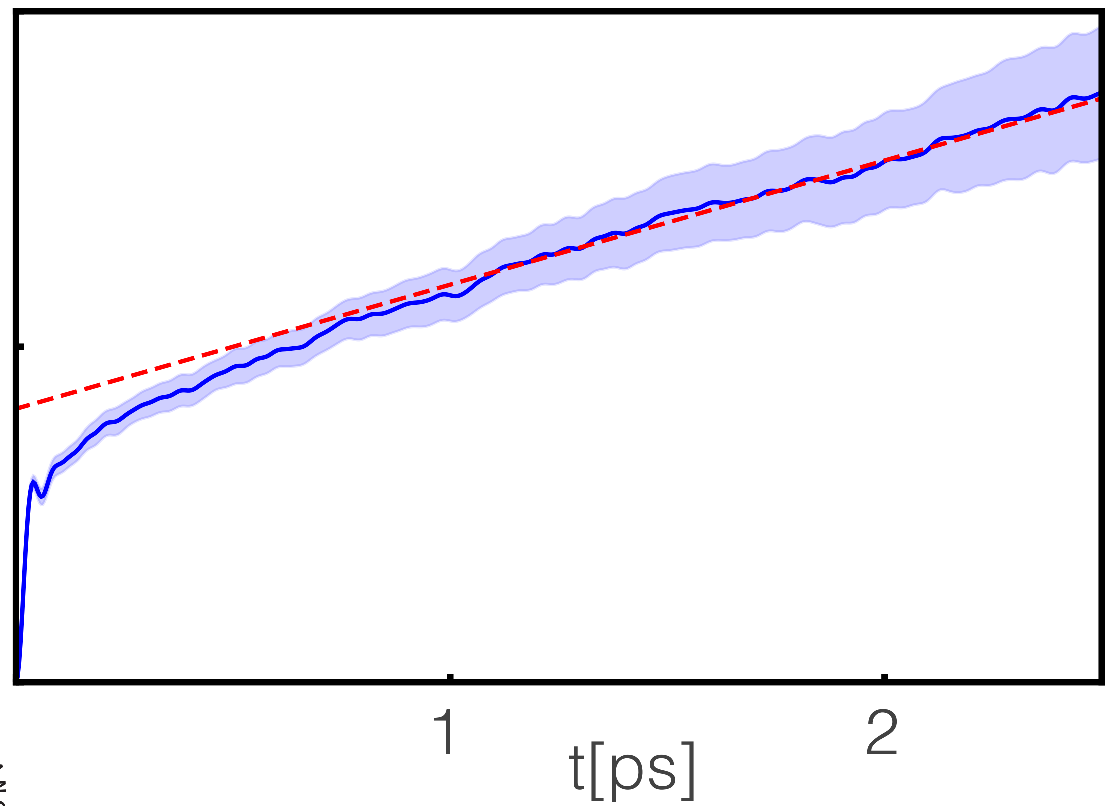
$$\frac{\mathsf{t}}{3Vk_BT^2}\int_0^{\mathsf{t}}\langle \mathbf{J}(\mathsf{t}')\cdot\mathbf{J}(0)\rangle d\mathsf{t}' \approx \frac{1}{6Vk_BT^2}\left\langle\left|\int_0^{\mathsf{t}}\mathbf{J}(\mathsf{t}')d\mathsf{t}'\right|^2\right\rangle$$

liquid (heavy) water

64 molecules, T=385 K



$$\frac{1}{3Vk_BT^2}\int_0^{\mathsf{t}} \langle \mathbf{J}(\mathsf{t}') \cdot \mathbf{J}(0)\rangle d\mathsf{t}'$$



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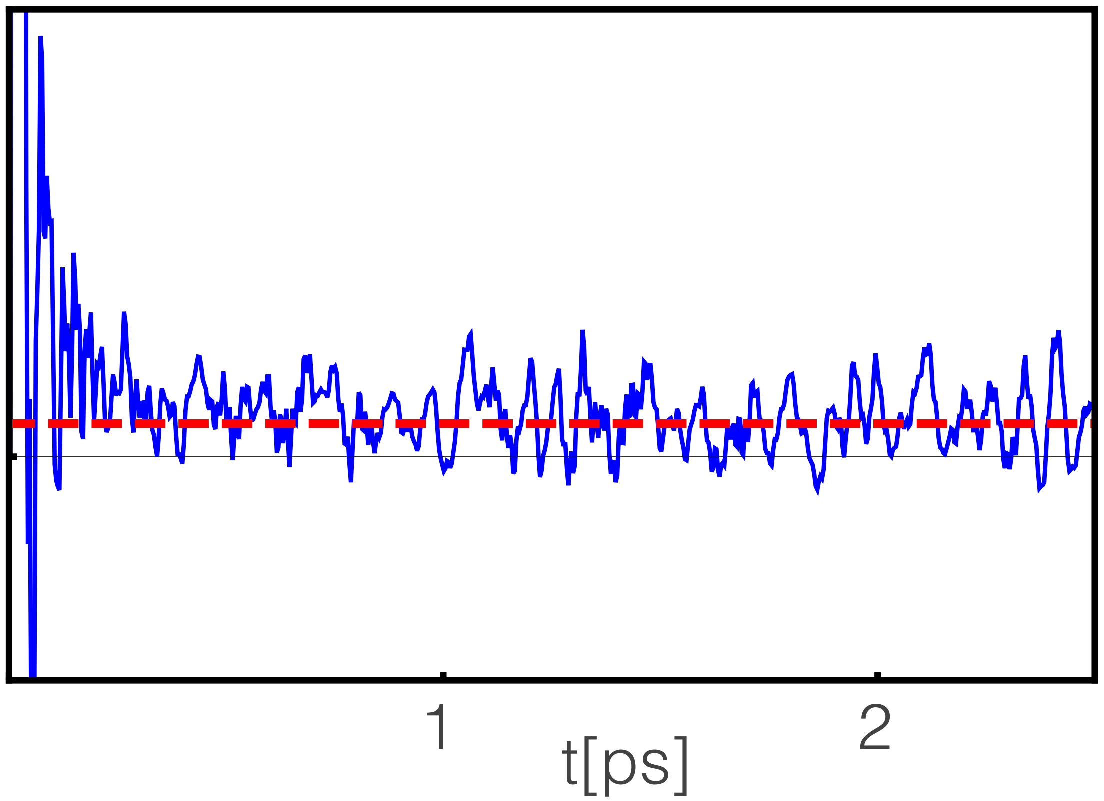
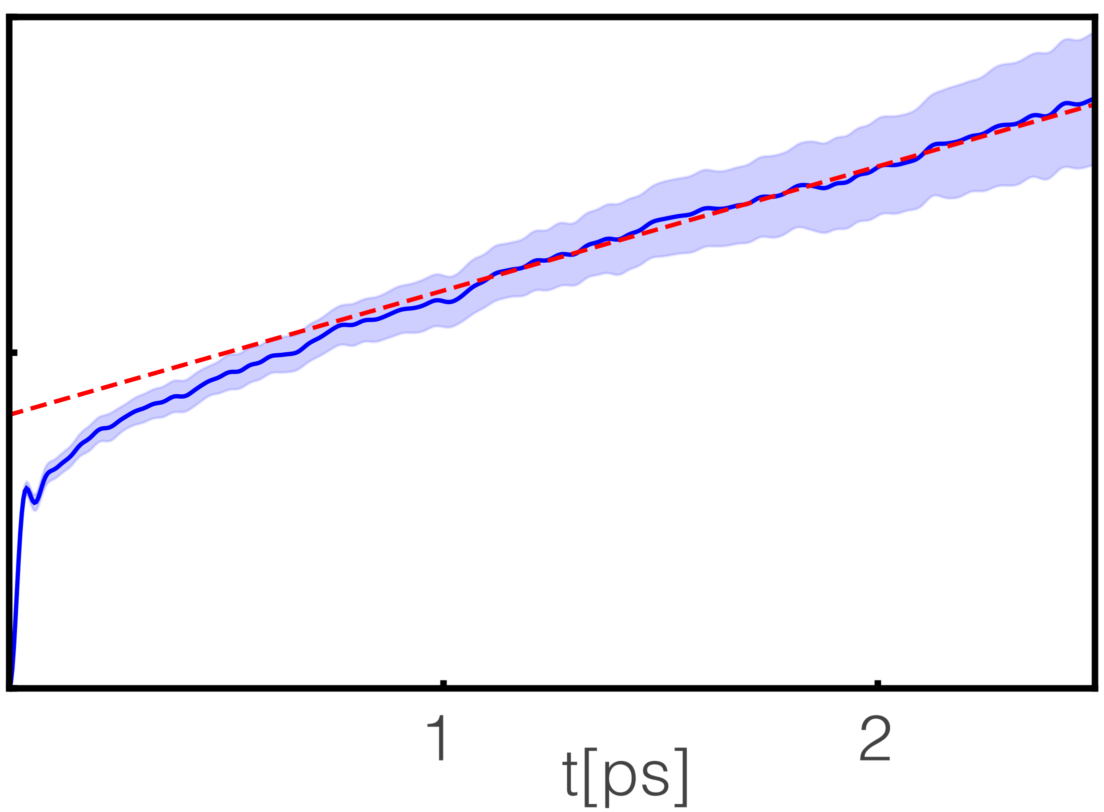




64 molecules, T=385 K

$$\frac{1}{3Vk_BT^2}\int_0^t \langle \mathbf{J}(t')\cdot\mathbf{J}(0)\rangle dt'$$

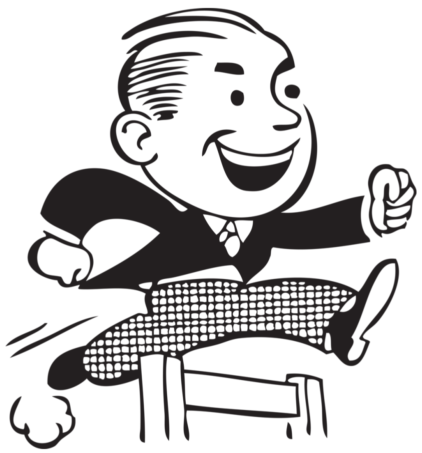
$$\kappa_{\text{DFT}} = 0.74 \pm 0.12\ \text{W}/(\text{mK})$$

$$\kappa_{\text{expt}} = 0.61 \quad (\text{light@AC})$$

$$\kappa_{\text{DFT}} = 0.60 \quad (\text{heavy@AC})$$

$$\frac{1}{6Vk_BT^2}\left\langle \left| \int_0^t \mathbf{J}(t')dt' \right|^2 \right\rangle$$

hurdles towards an ab initio Green-Kubo theory



PRL **104,** 208501 (2010) PHYSICAL REVIEW LETTERS week ending 21 MAY 2010

Thermal Conductivity of Periclase (MgO) from First Principles

Stephen Stackhouse, Lars Stixrude, and Bijaya B. Karki

sensitive to the form of the potential. The widely used Green-Kubo relation [14] does not serve our purposes, because in first-principles calculations it is impossible to uniquely decompose the total energy into individual contributions from each atom.

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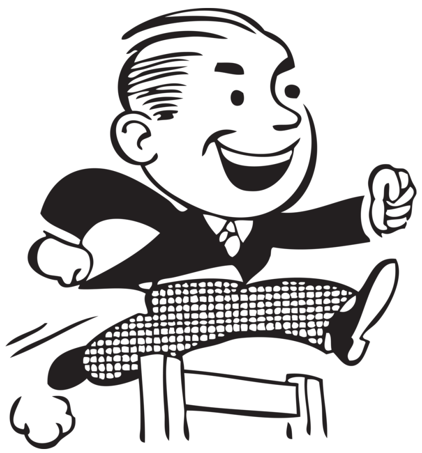

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PRL **118,** 175901 (2017) PHYSICAL REVIEW LETTERS week ending 28 APRIL 2017

Ab Initio **Green-Kubo Approach for the Thermal Conductivity of Solids**

Christian Carbogno, Rampi Ramprasad, and Matthias Scheffler

ulations: Because of the limited time scales accessible in aiMD runs, thermodynamic fluctuations dominate the HFACF, which in turn prevents a reliable and numerically stable assessment of the thermal conductivity via Eq. (2).

separating wheat from chaff

$$\kappa \propto \int_0^\infty C(t)dt$$

$$C(t) = \langle J(t)J(0)\rangle$$

$$\kappa \propto S(\omega = 0)$$

$$S(\omega) = \int_{-\infty}^{\infty} C(t)\mathrm{e}^{-i\omega t}dt$$

separating wheat from chaff

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$$\kappa \propto S(\omega = 0) \qquad S(\omega) = \int_{-\infty}^{\infty} C(t)\mathrm{e}^{-i\omega t}dt$$

the Wiener-Khintchine theorem

$$S(\omega) = \lim_{T\to\infty} \left\langle \left| \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} J(t)\mathrm{e}^{i\omega t} \right|^2 \right\rangle$$

separating wheat from chaff

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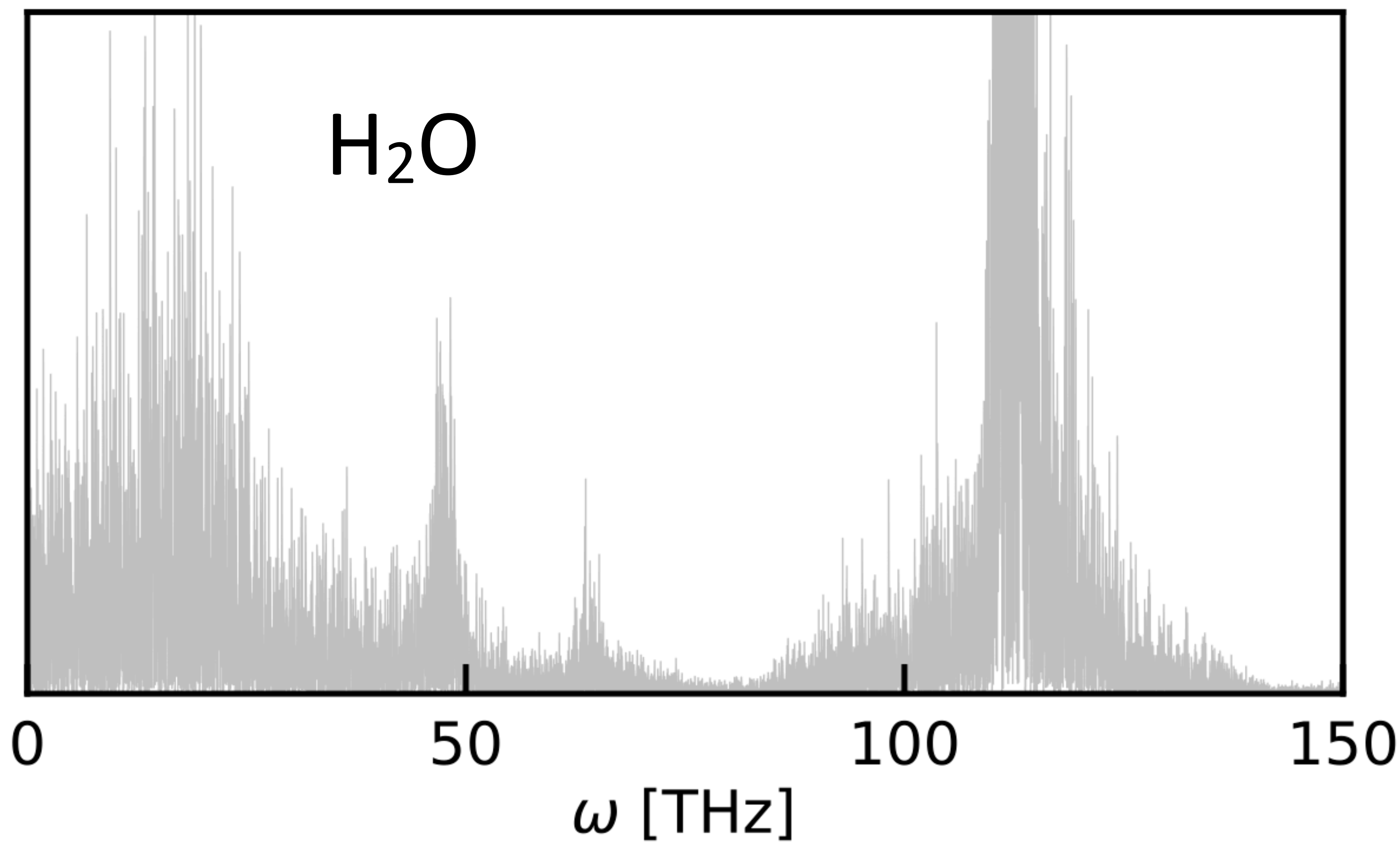
in practice:

$$S\left(\omega_k\right) = \frac{\epsilon}{N} \left\langle \left| \sum_{n=0}^{N-1} J_n \mathrm{e}^{-i\frac{2\pi nk}{N}} \right|^2 \right\rangle$$

separating wheat from chaff

$$\hat{S}(k) = \frac{\epsilon}{N}\left|\tilde{J}(k)\right|^2$$
$$= \frac{1}{2}S(\omega_k) \times \chi_2^2$$



separating wheat from chaff

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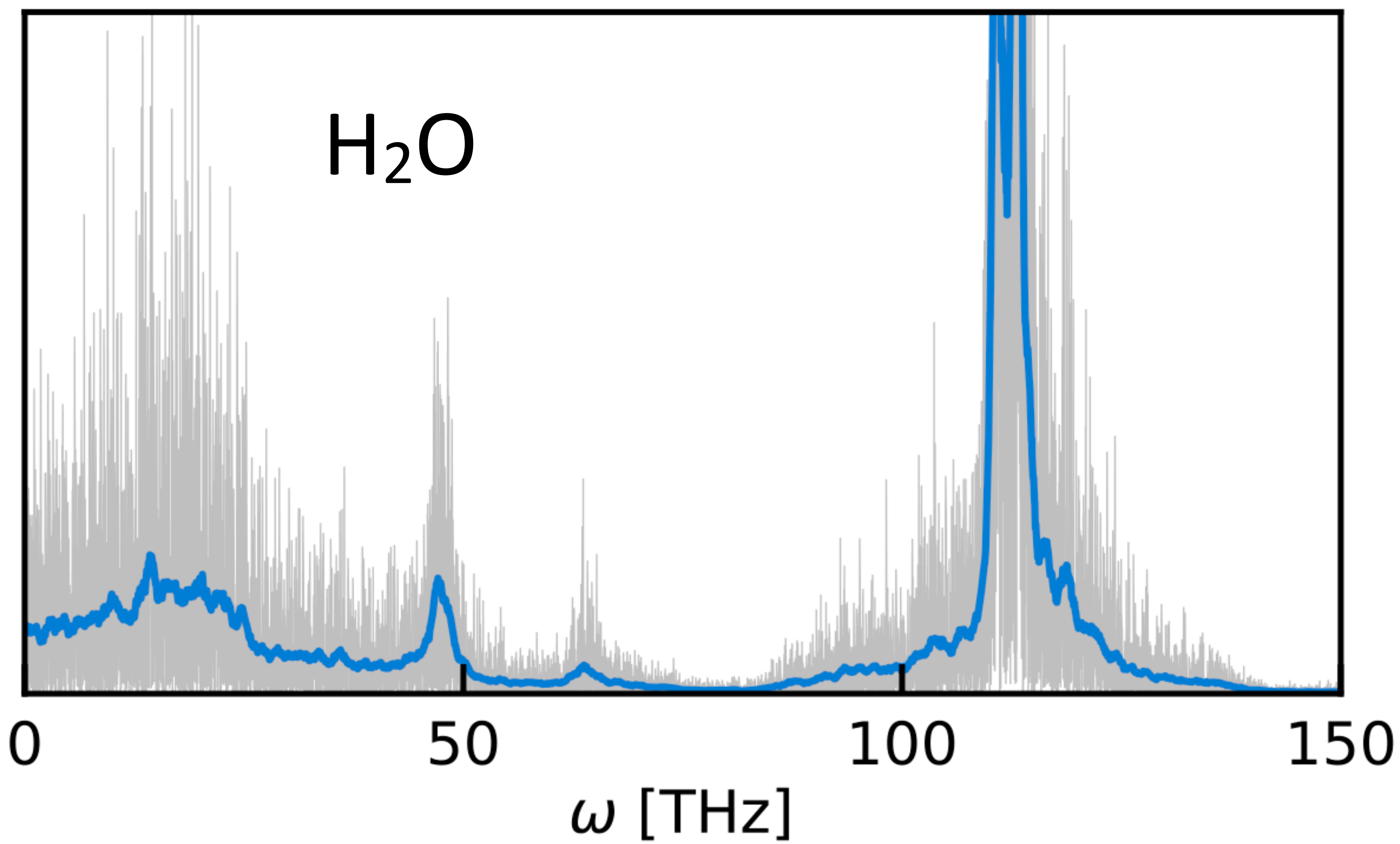

separating wheat from chaff

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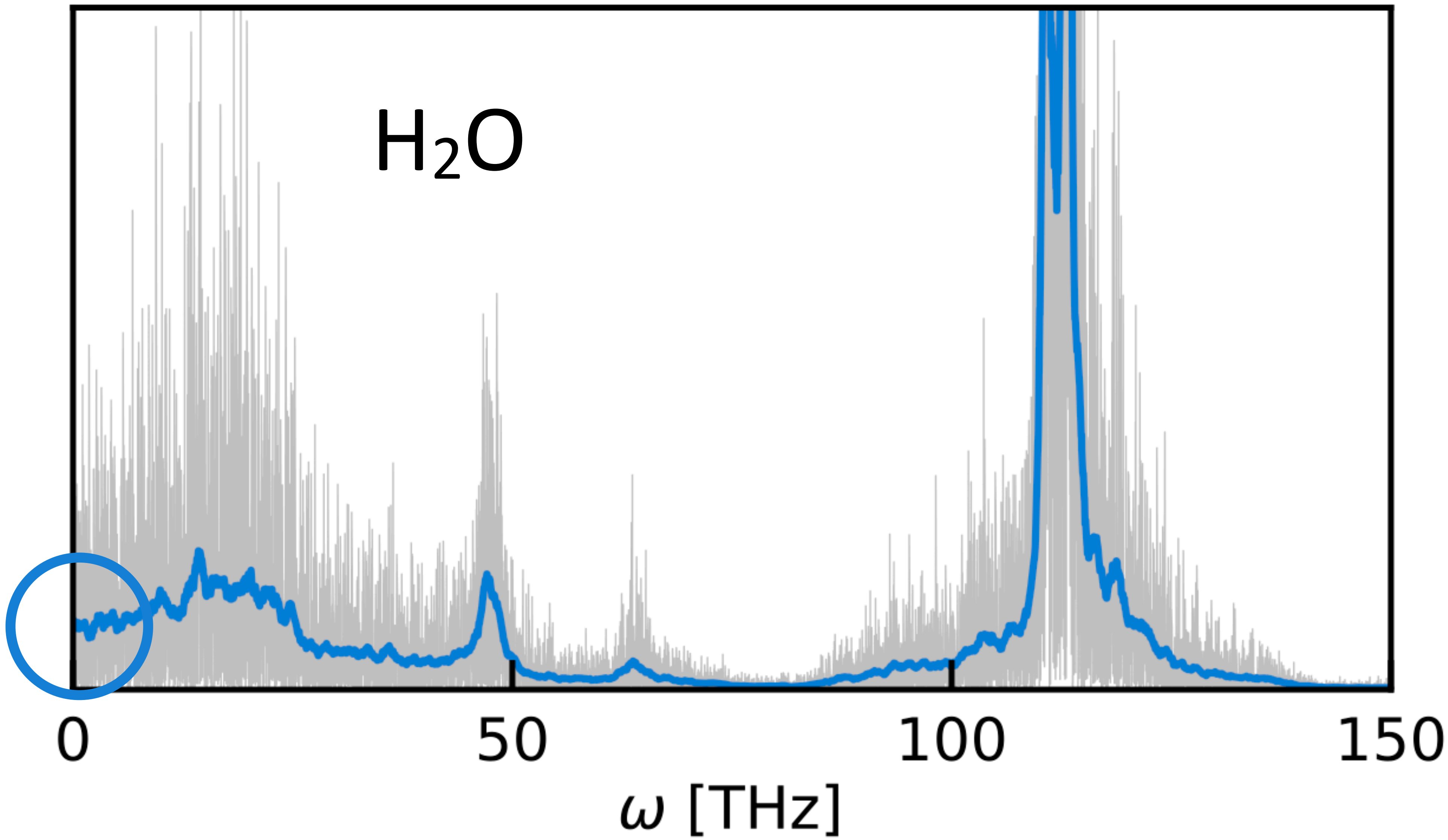
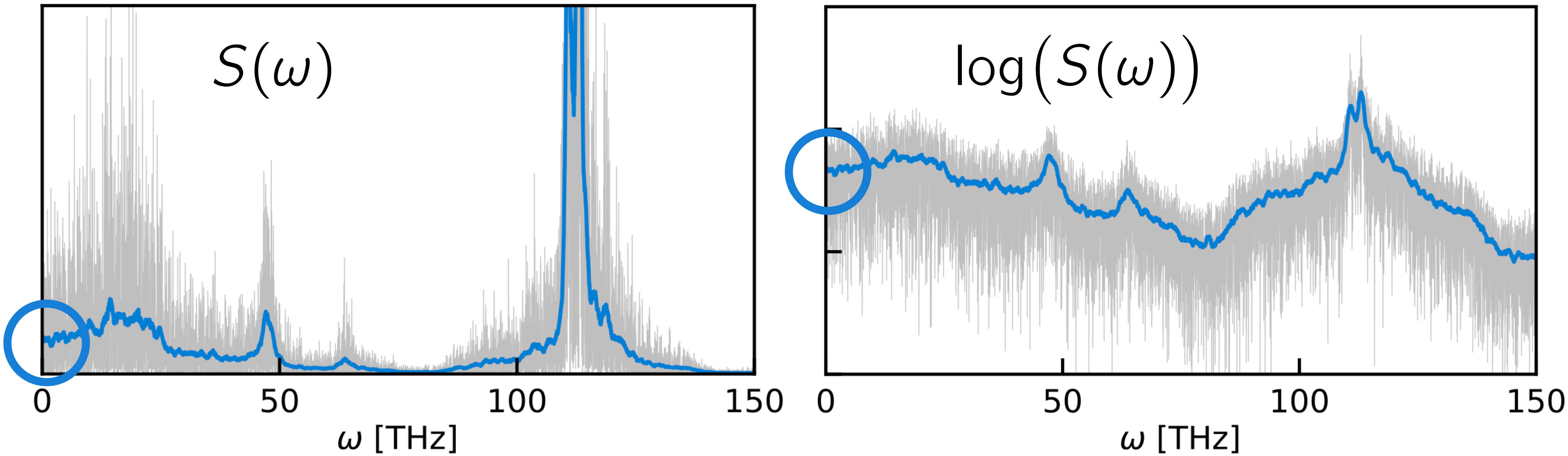


separating wheat from chaff

$$\hat{S}(k) = S(\omega_k)\hat{\xi}_k$$

$$\log\left(\hat{S}(k)\right) = \log\left(S(\omega_k)\right) + \log\left(\hat{\xi}_k\right)$$



separating wheat from chaff

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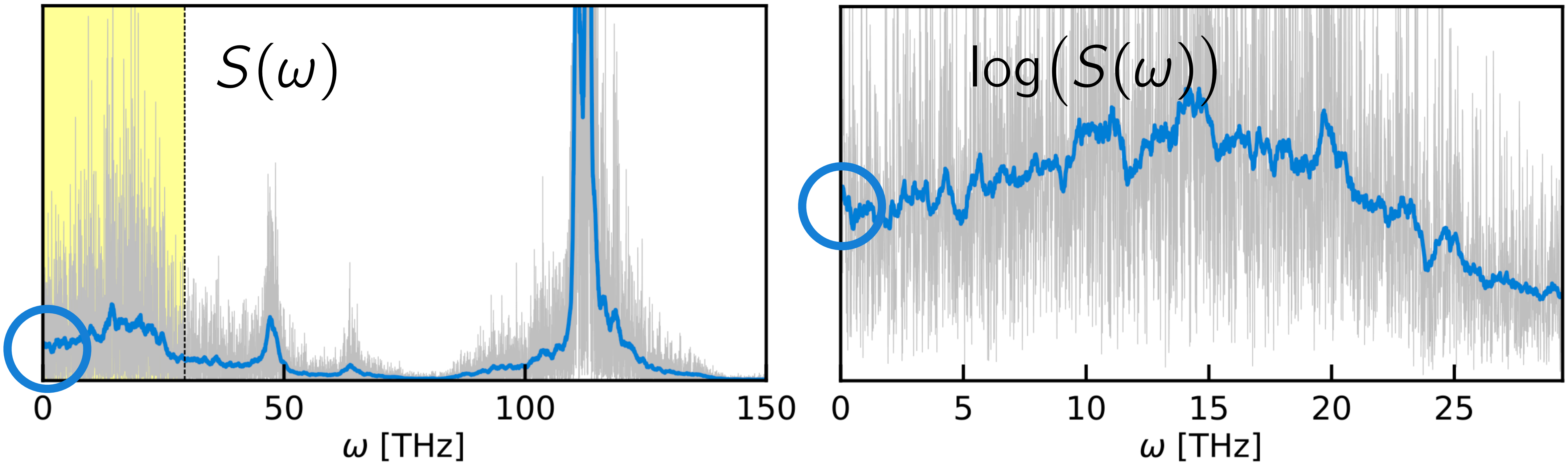
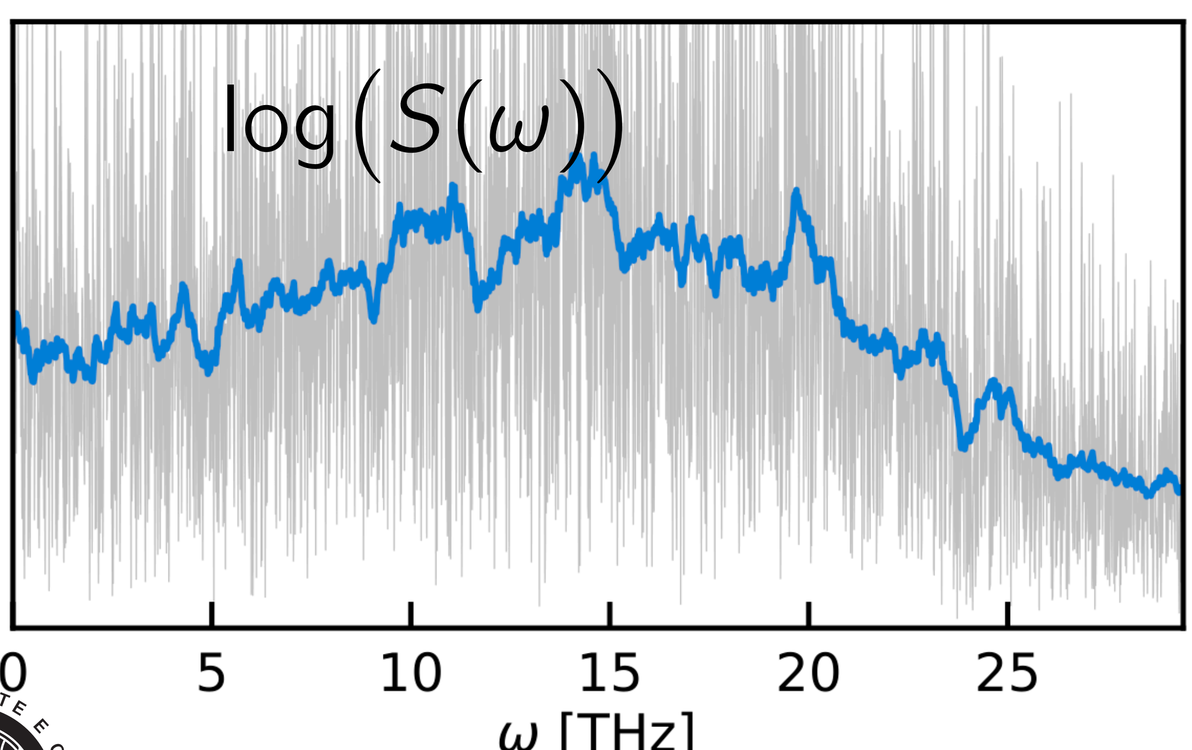
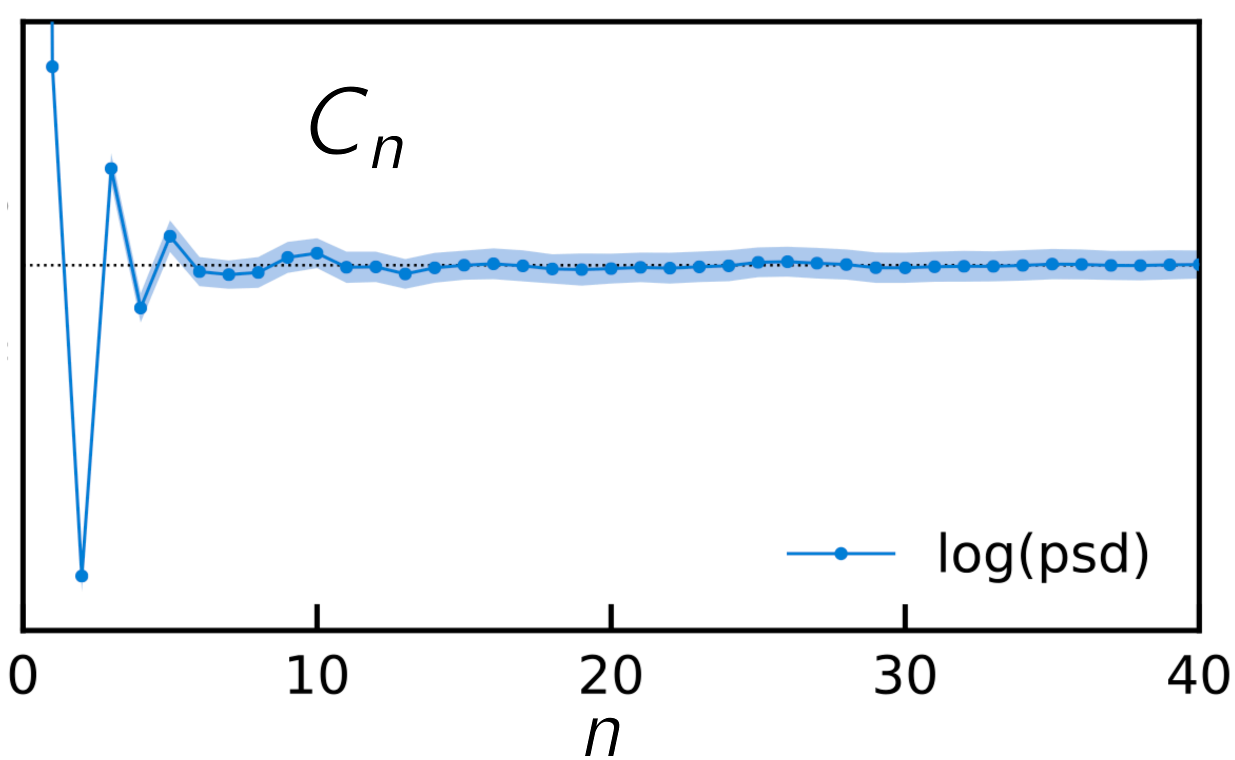


separating wheat from chaff

$$\log\left(\hat{S}(k)\right) = \log\left(S(\omega_k)\right) + \log\left(\hat{\xi}_k\right)$$

$$\frac{1}{N}\sum_{k=0}^{N-1} \log\left(\hat{S}(k)\right) \mathrm{e}^{-i\frac{2\pi kn}{N}} = C_n + \text{white noise}$$





separating wheat from chaff

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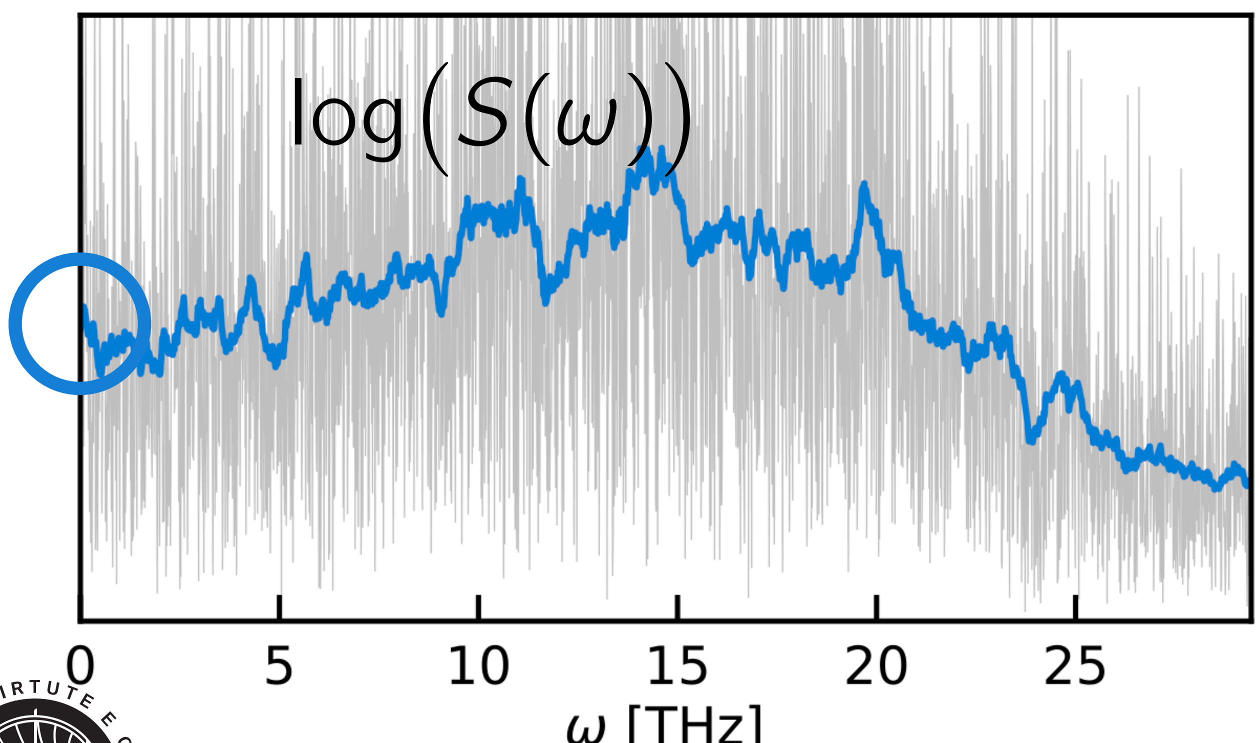

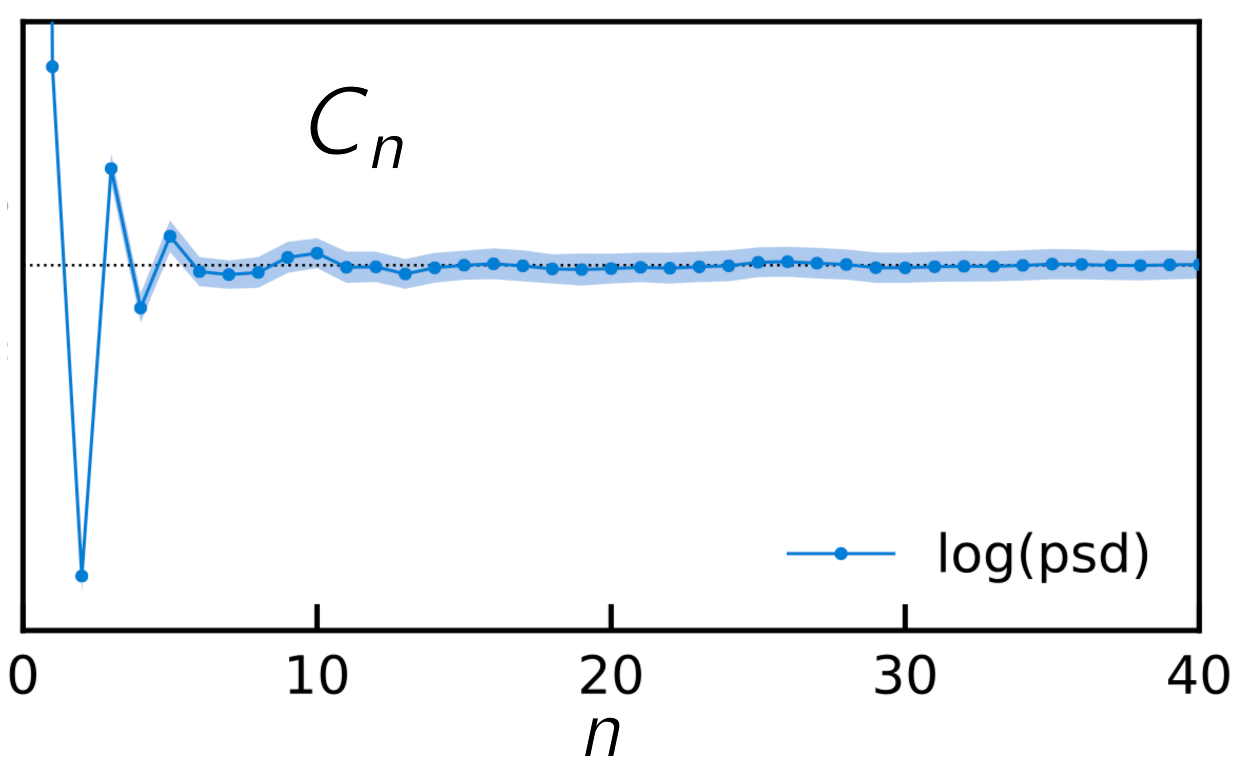

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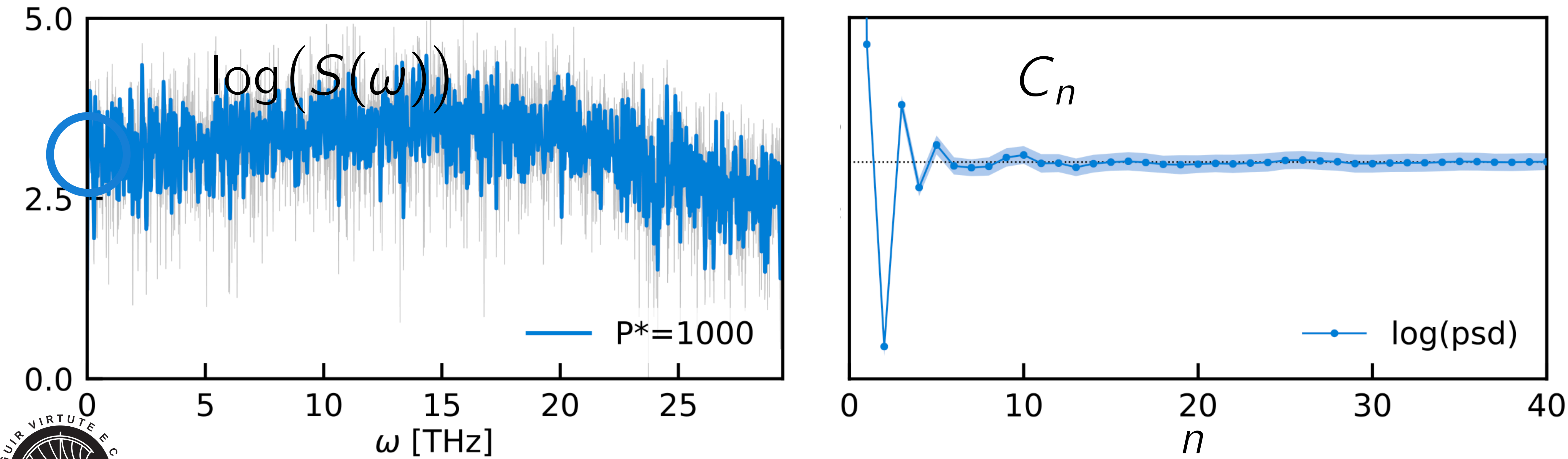

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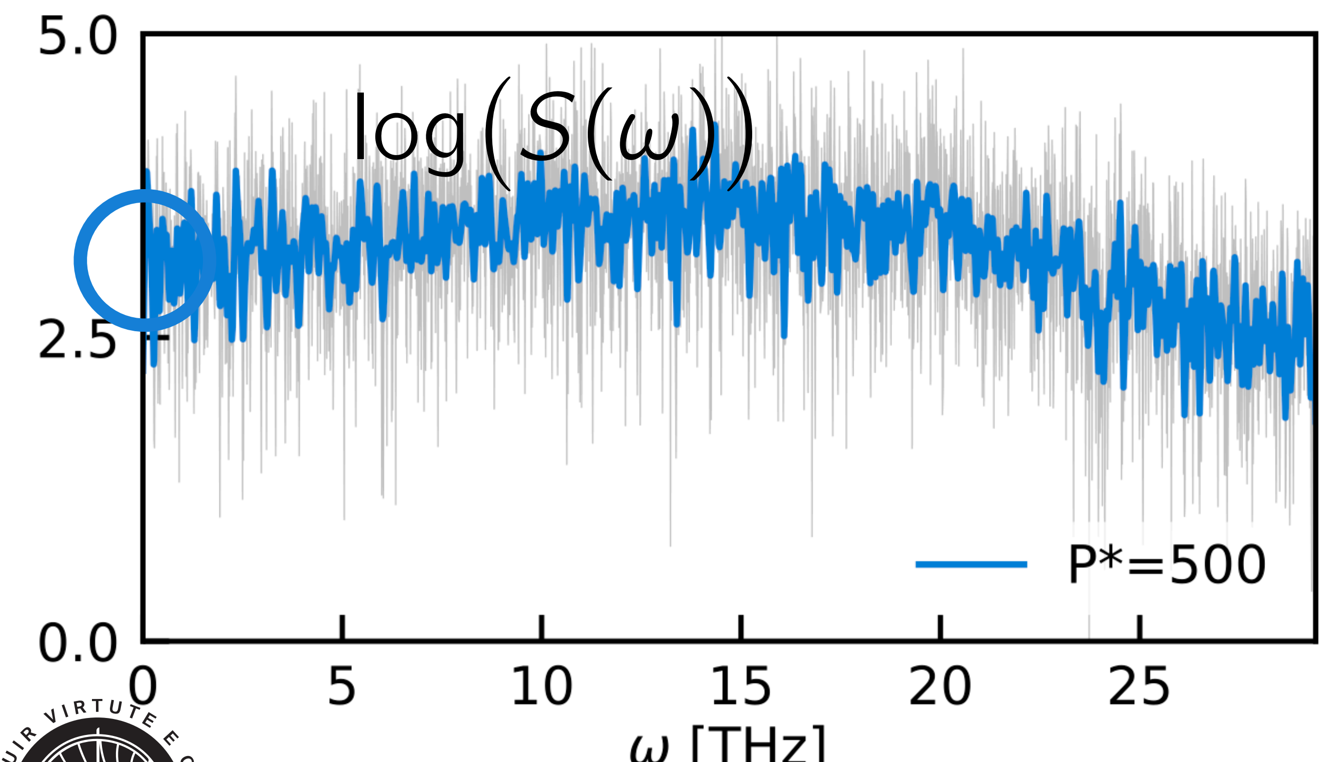

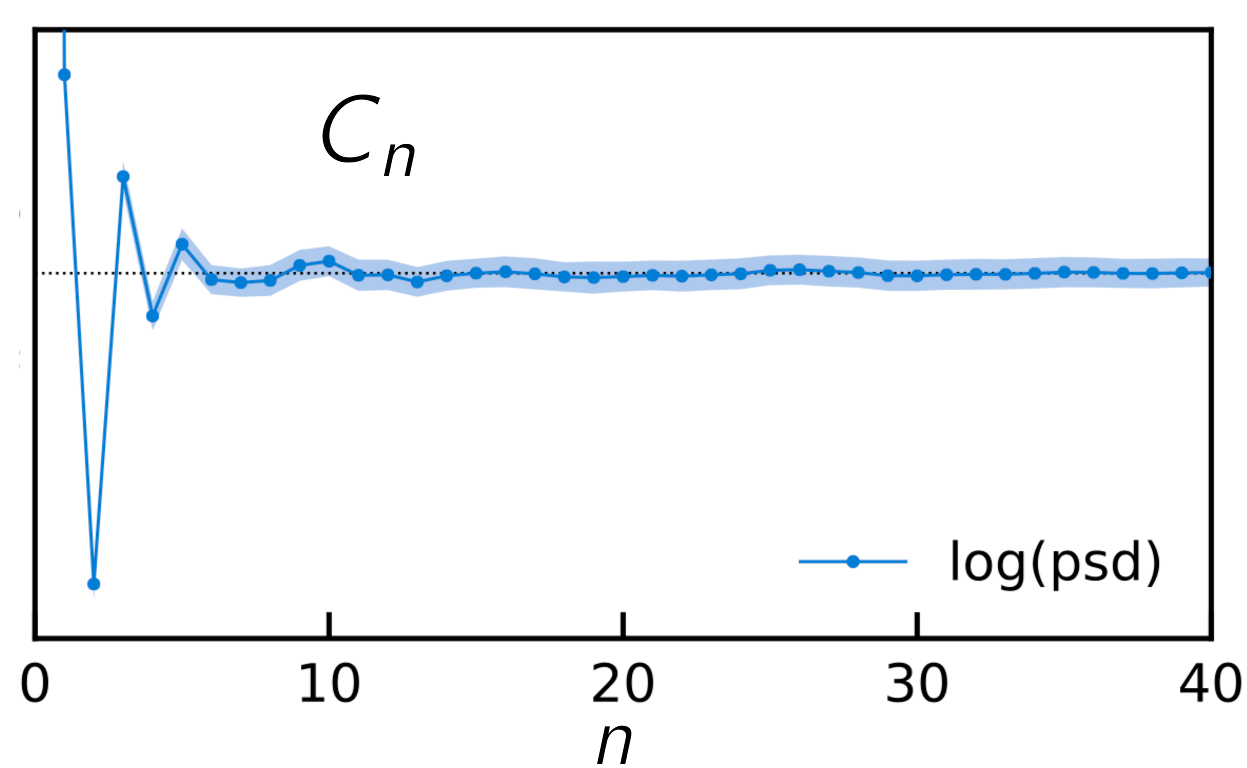

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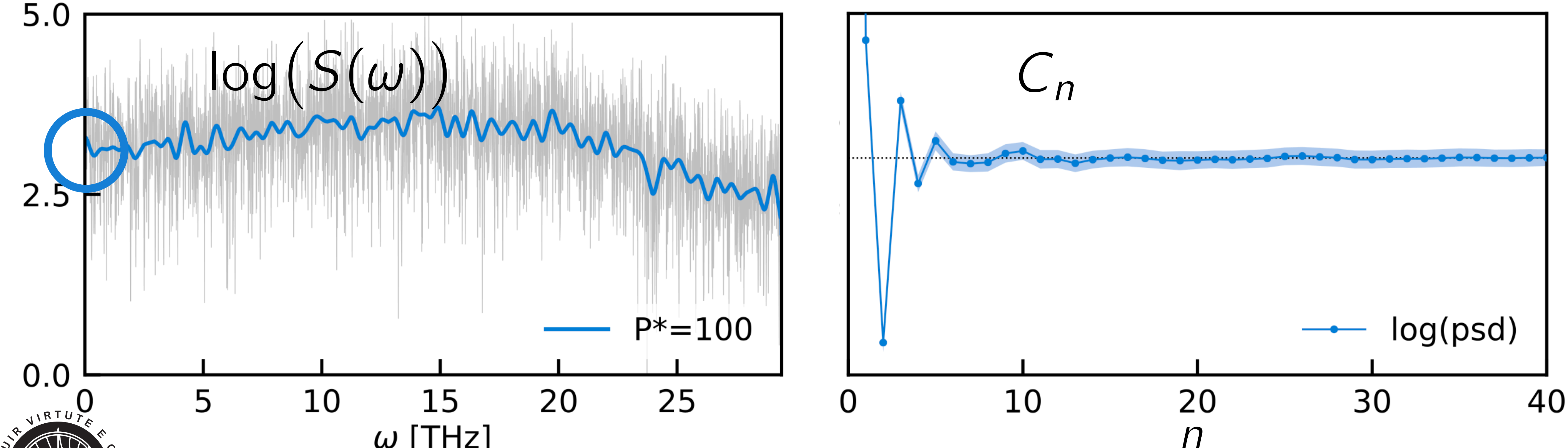

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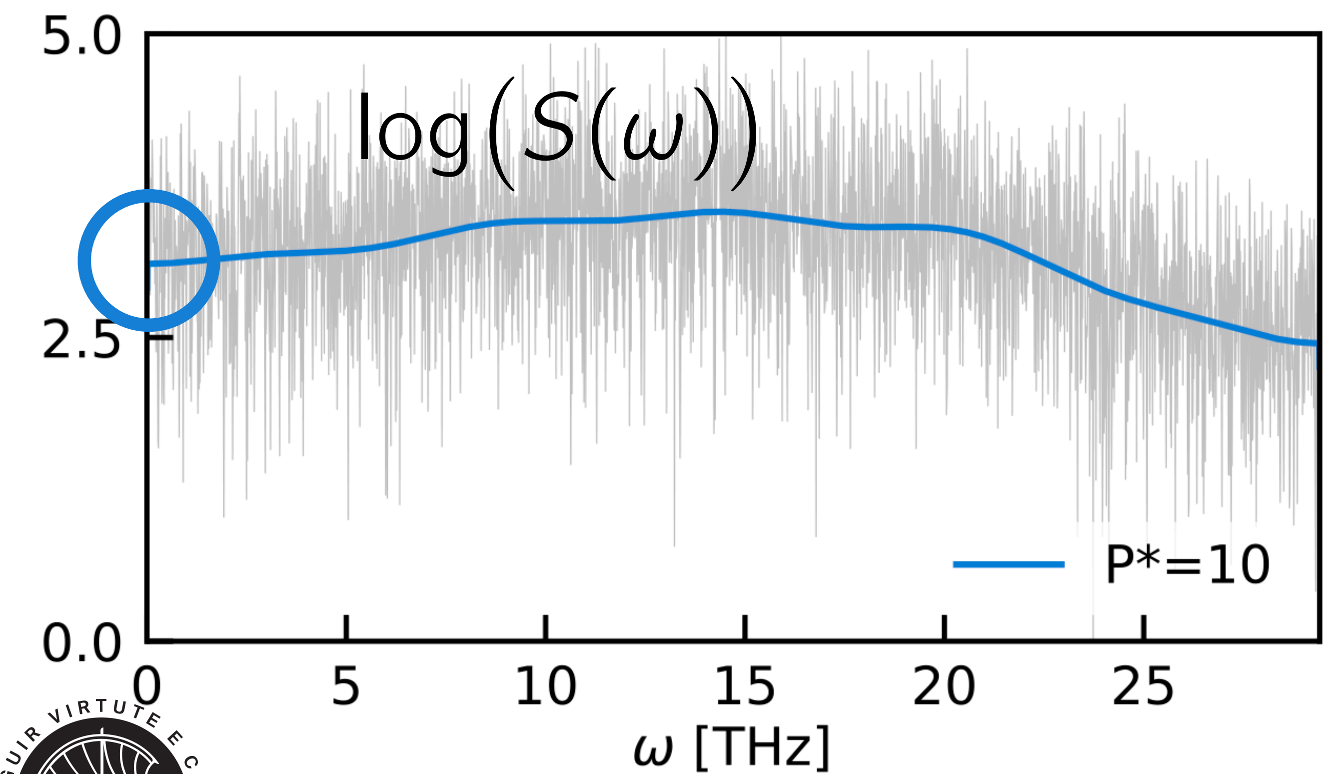

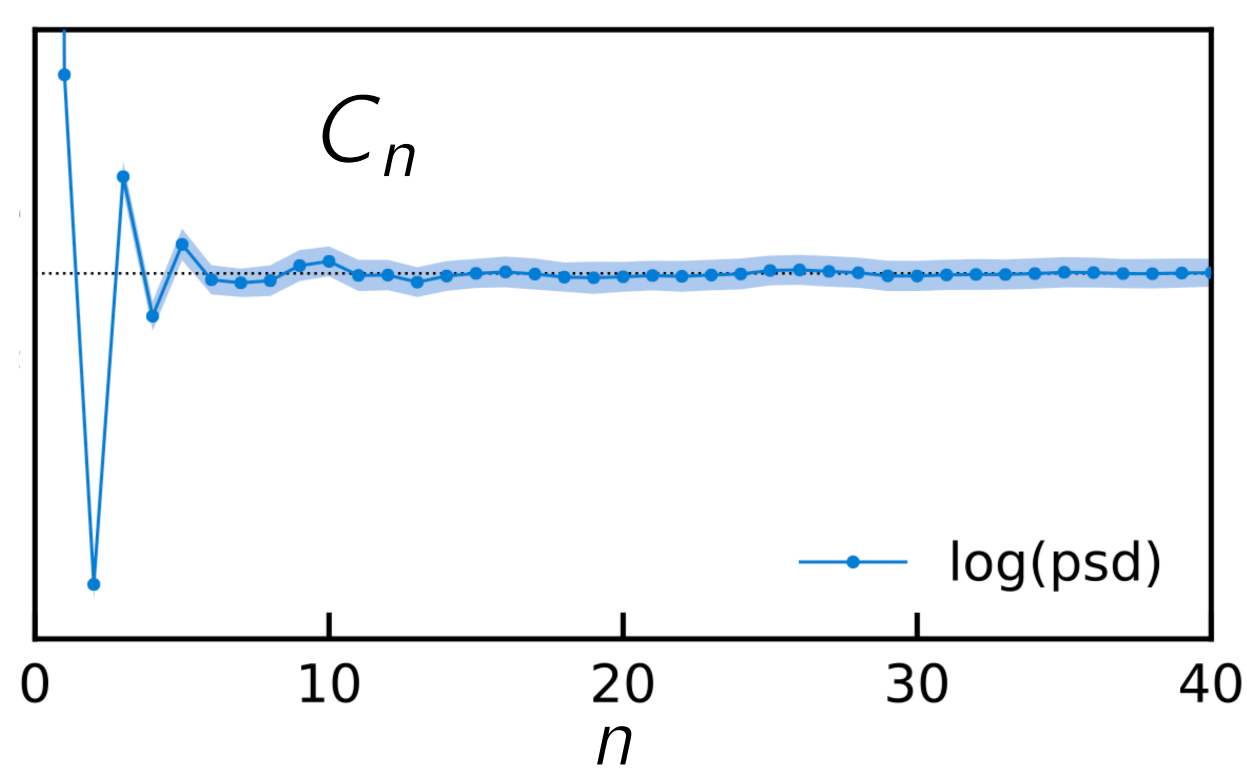

separating wheat from chaff

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optimal number of coefficients, to be determined

$$\log(\kappa) = \lambda + C_0 + 2\sum_{n=1}^{P^*-1} C_n \pm \sigma\sqrt{\frac{4P^* - 2}{N^*}}$$

constants independent of the time series being sampled

separating wheat from chaff

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$$\frac{\Delta\kappa}{\kappa} = \begin{cases} \text{Ar} & (100 \text{ ps}) & 10\ \% \\ \text{H}_2\text{O} & (100 \text{ ps}) & 5\ \% \\ \text{a-SiO}_2 & (100 \text{ ps}) & 12\ \% \\ \text{c-MgO} & (500 \text{ ps}) & 15\ \% \end{cases}$$

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separating wheat from chaff

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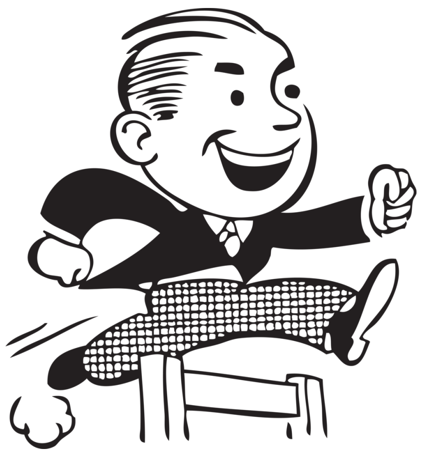
an analogous methodology can be applied to multi-component fluids

hurdles towards an ab initio Green-Kubo theory

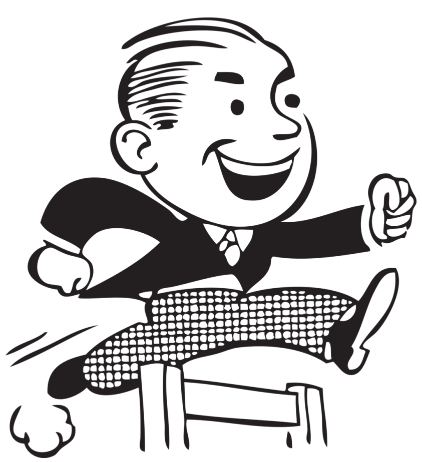


PRL **104,** 208501 (2010) PHYSICAL REVIEW LETTERS week ending 21 MAY 2010

Thermal Conductivity of Periclase (MgO) from First Principles

Stephen Stackhouse, Lars Stixrude, and Bijaya B. Karki

sensitive to the form of the potential. The widely used Green-Kubo relation [14] does not serve our purposes, because in first-principles calculations it is impossible to uniquely decompose the total energy into individual contributions from each atom.



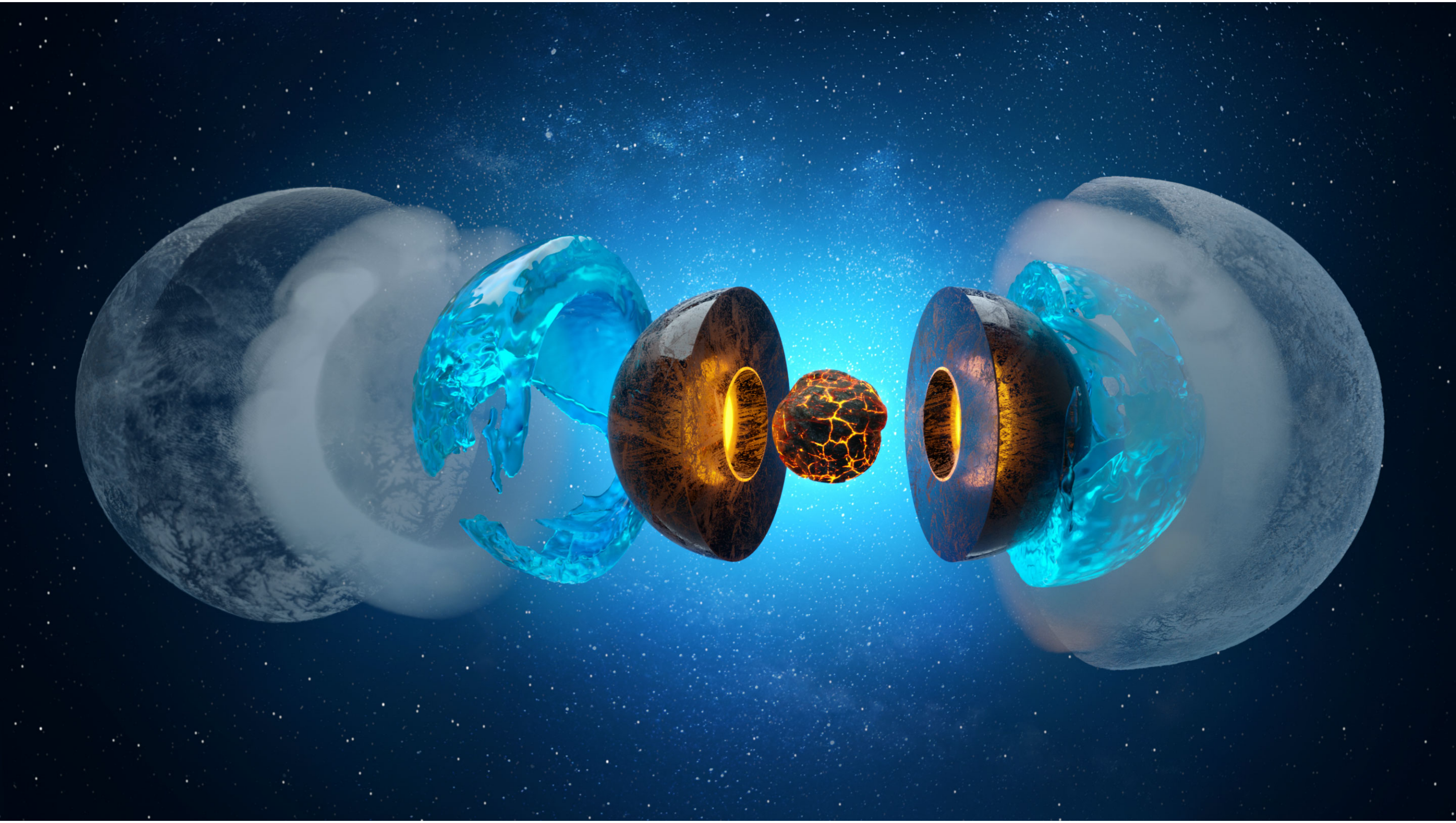
PRL **118,** 175901 (2017) PHYSICAL REVIEW LETTERS week ending 28 APRIL 2017

***Ab Initio* Green-Kubo Approach for the Thermal Conductivity of Solids**

Christian Carbogno, Rampi Ramprasad, and Matthias Scheffler

ulations: Because of the limited time scales accessible in aiMD runs, thermodynamic fluctuations dominate the HFACF, which in turn prevents a reliable and numerically stable assessment of the thermal conductivity via Eq. (2).

H_2O in Uranus



from quantamazine.org

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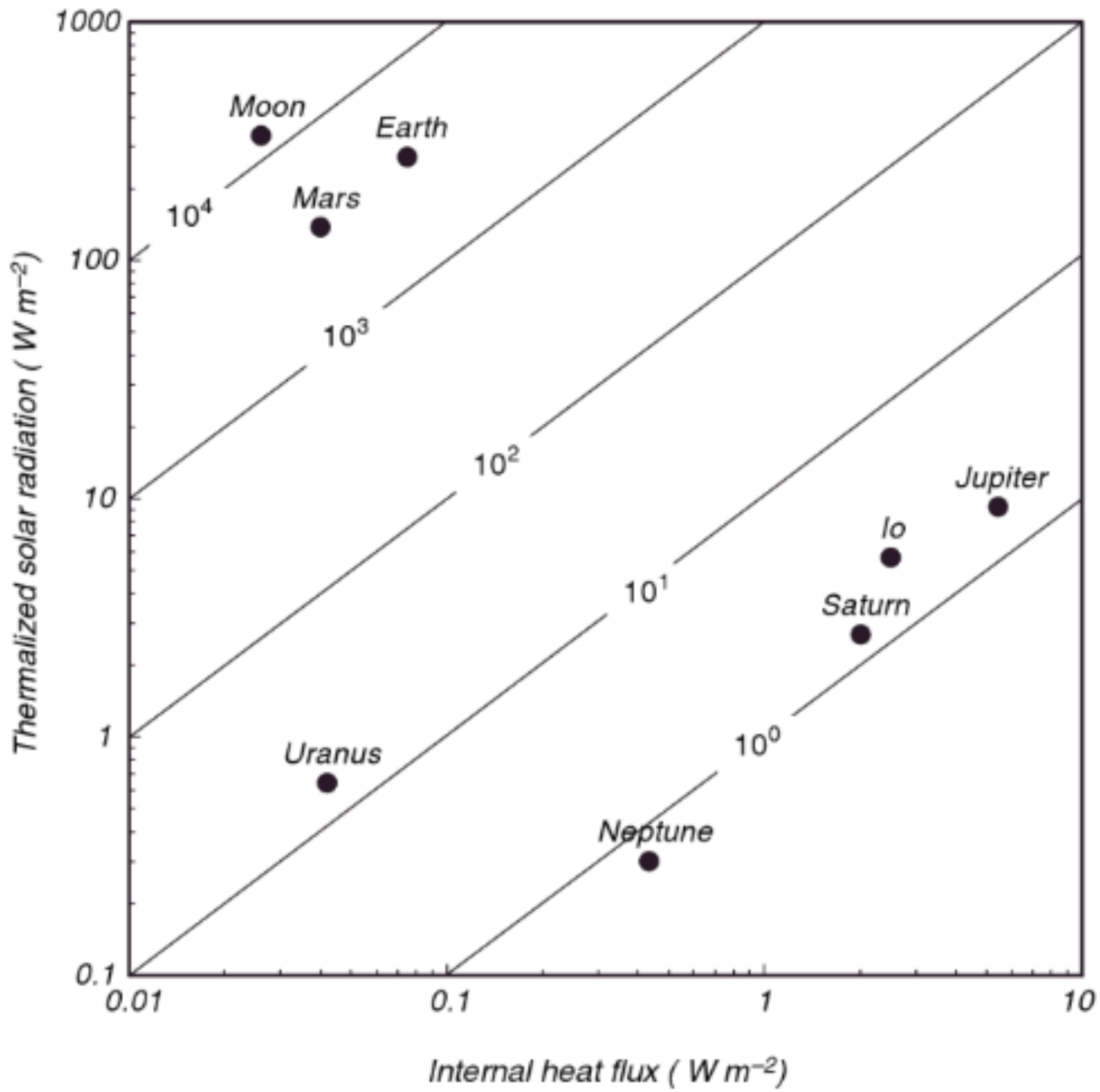

from: Patiño Douce, *Thermodynamics of the Earth and Planets*, Cambridge University Press, Cambridge & New York (2011)

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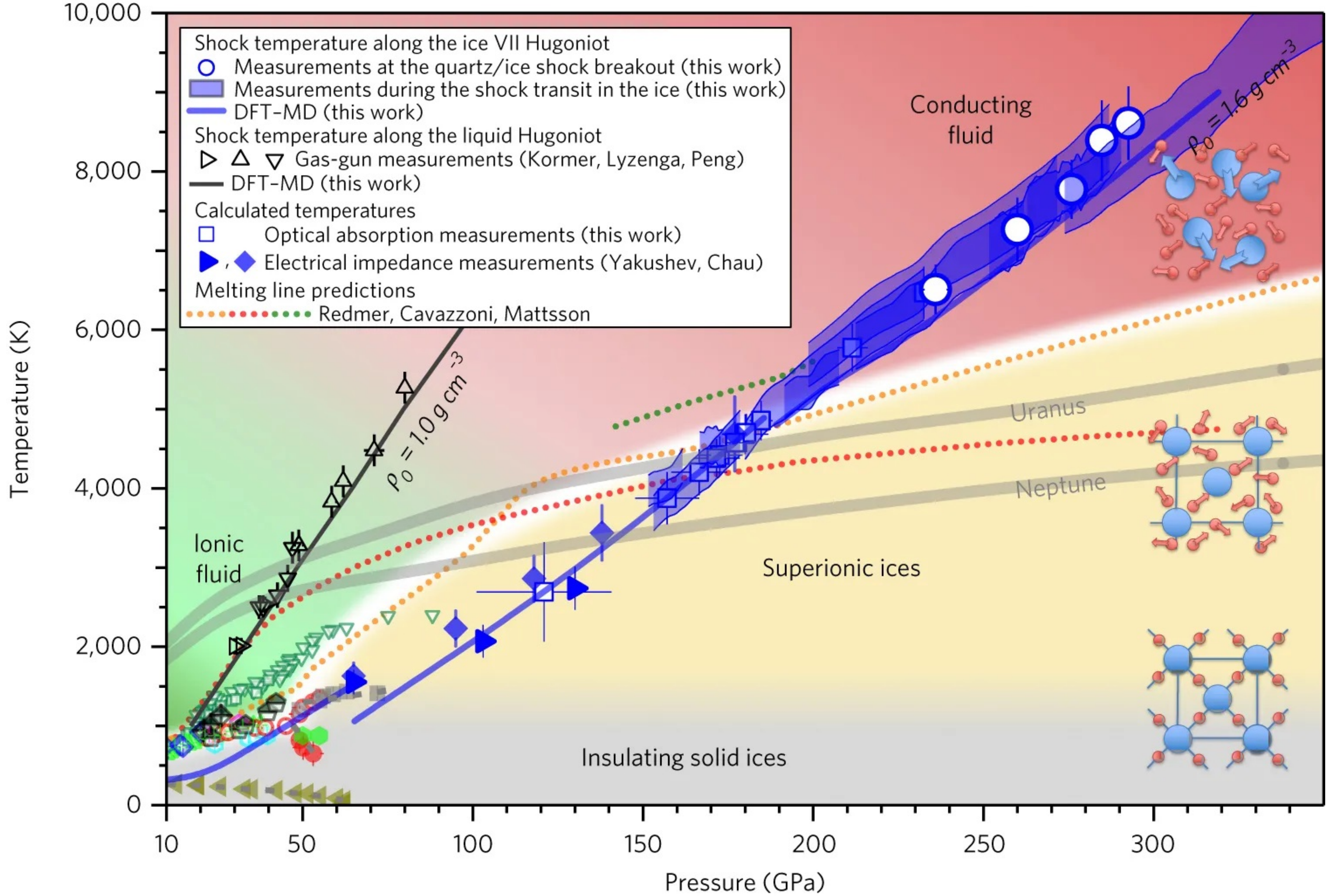

Millot, M., Hamel, S., Rygg, J.R. et al., Nature Phys **14**, 297–302 (2018)

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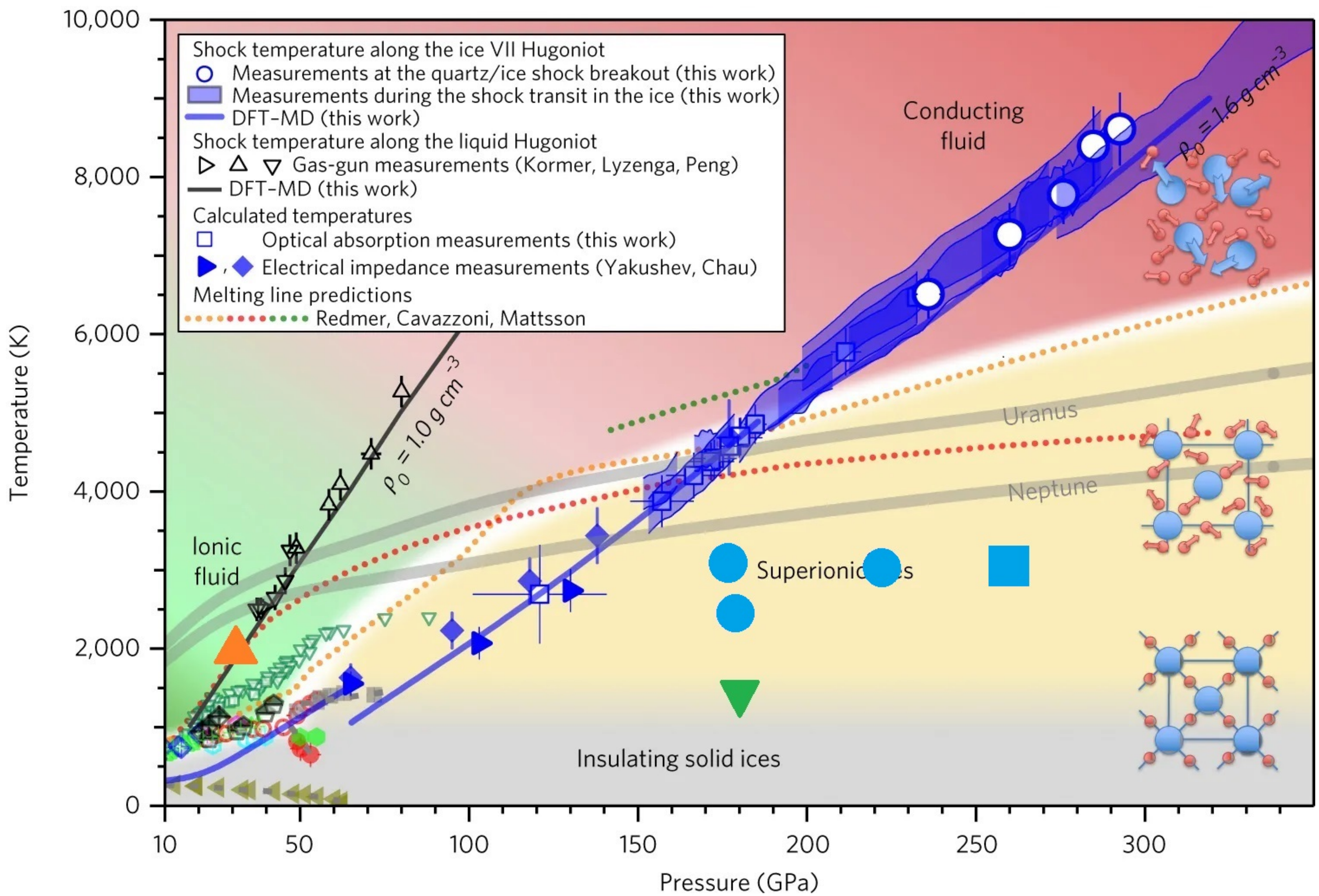

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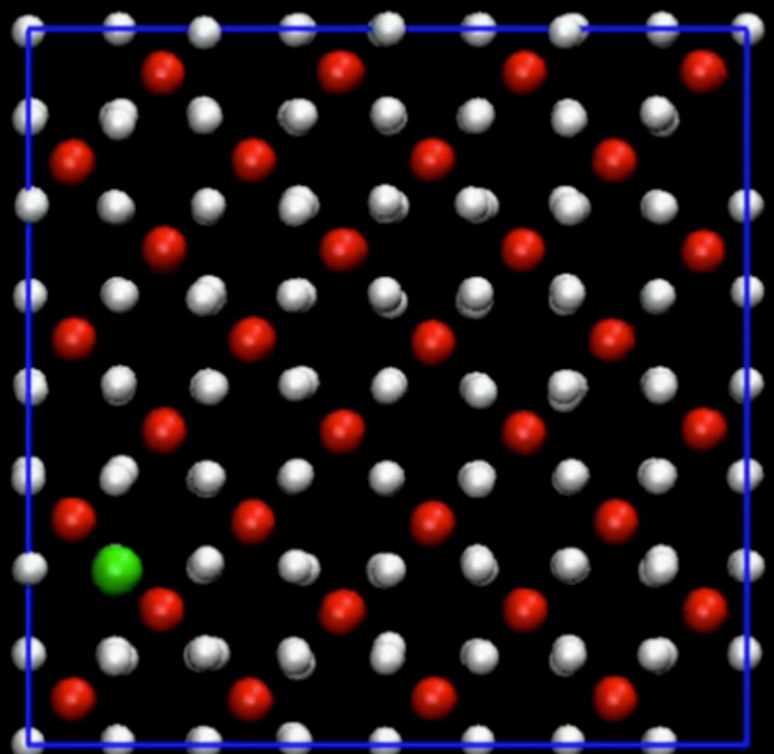
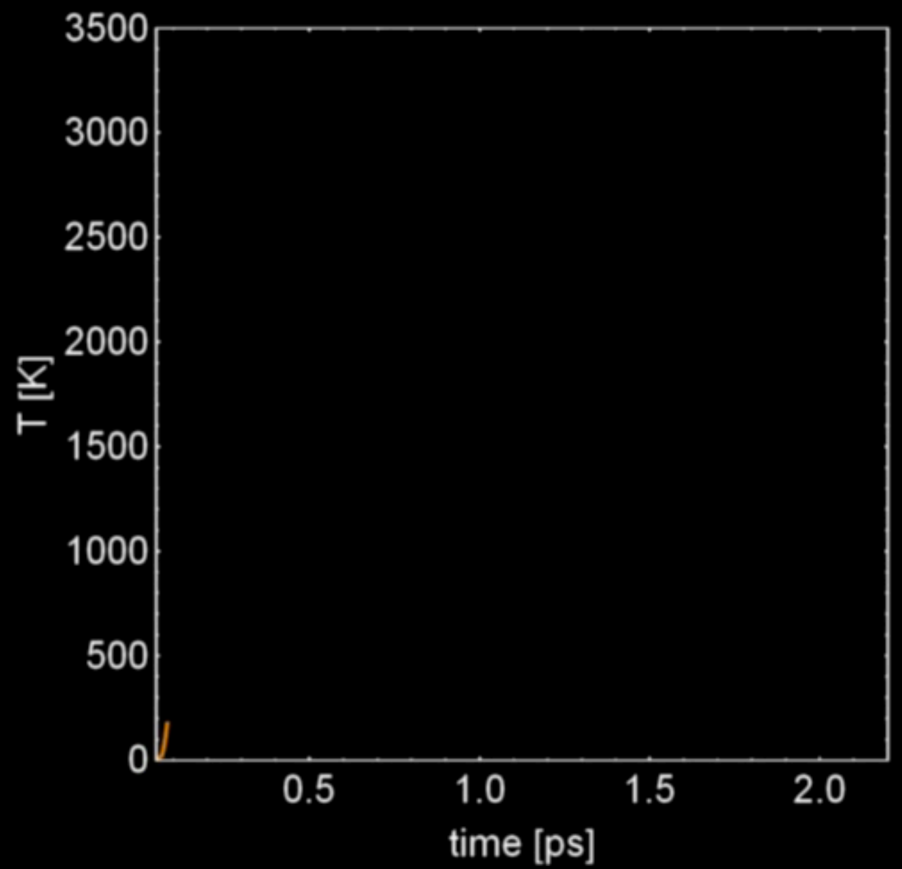
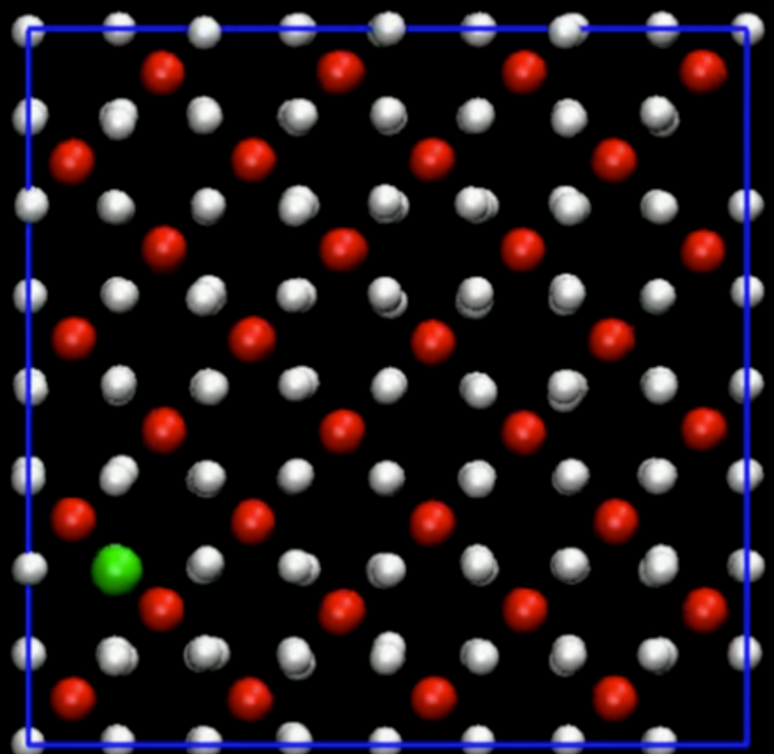
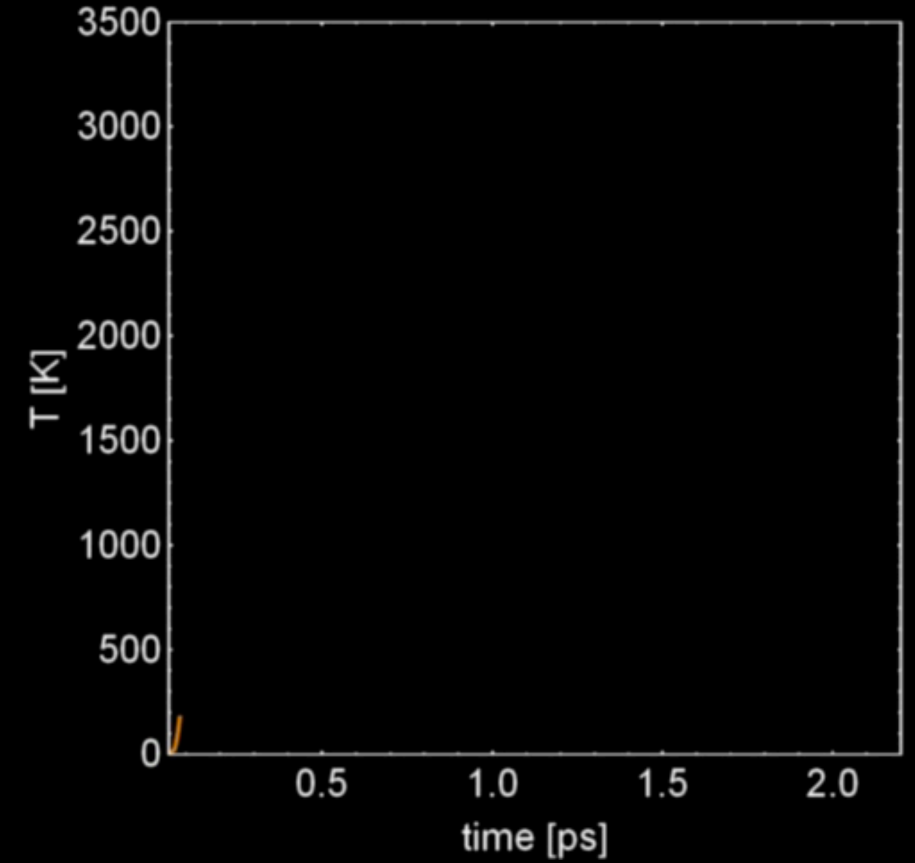




P = 175 GPa

H_2O in Uranus

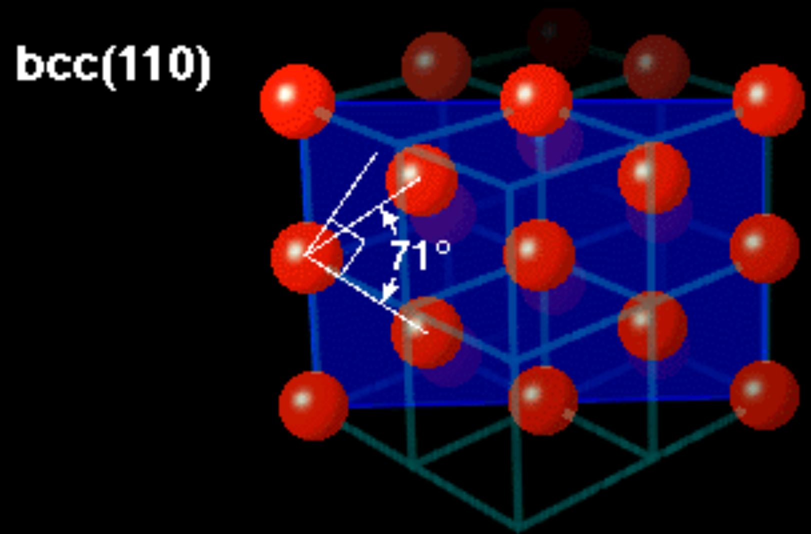


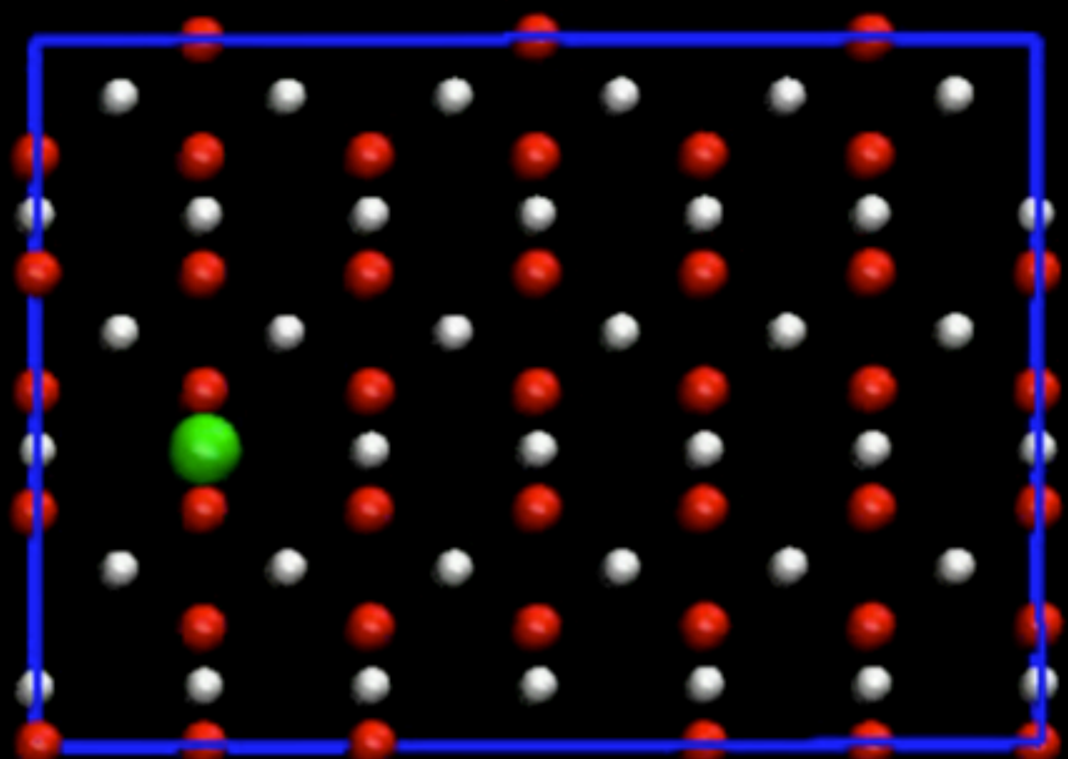


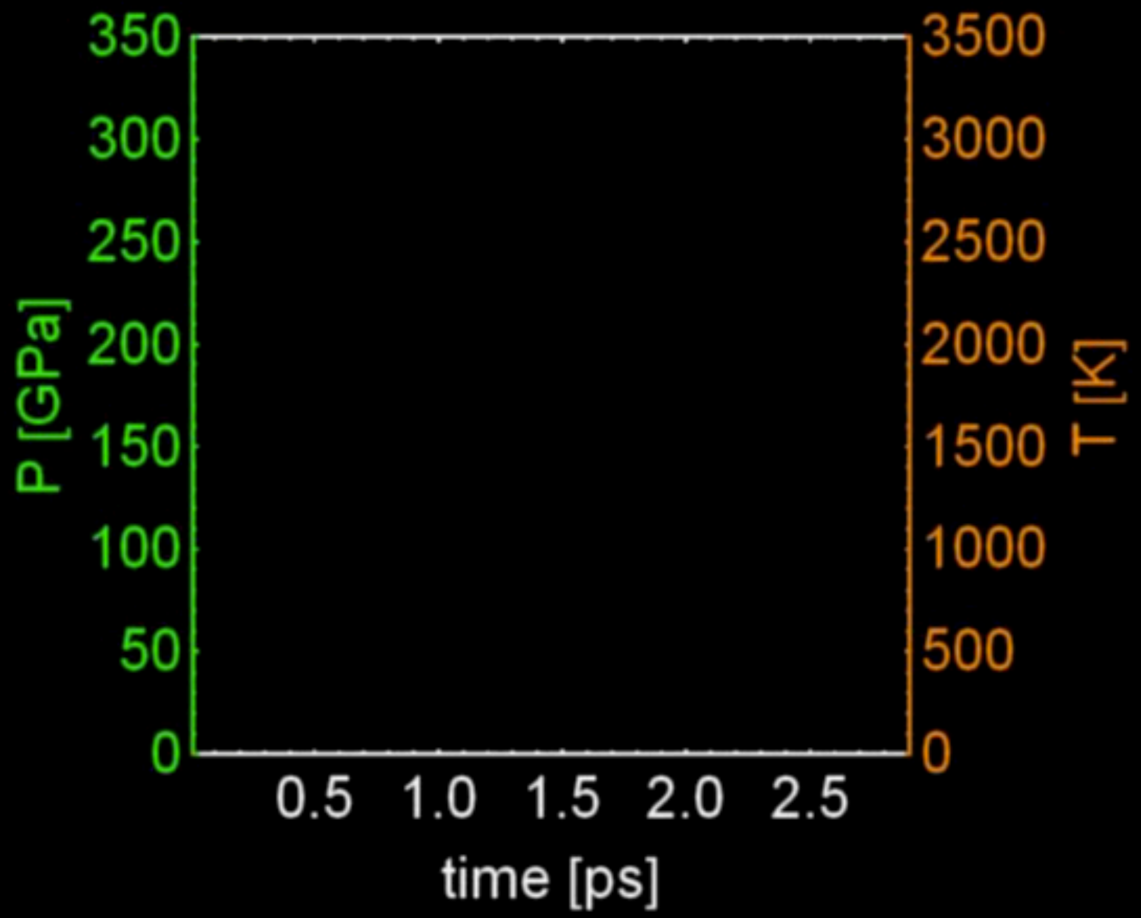
P = 175 GPa

T = 3000 K

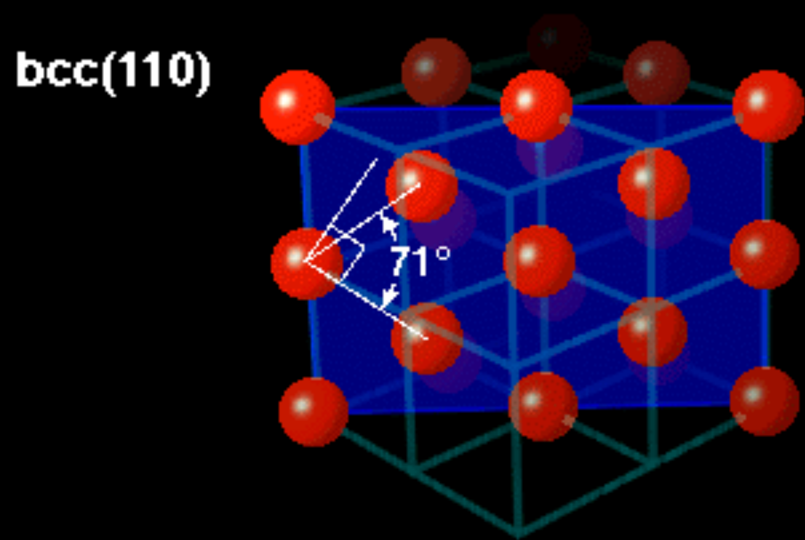
H_2O in Uranus

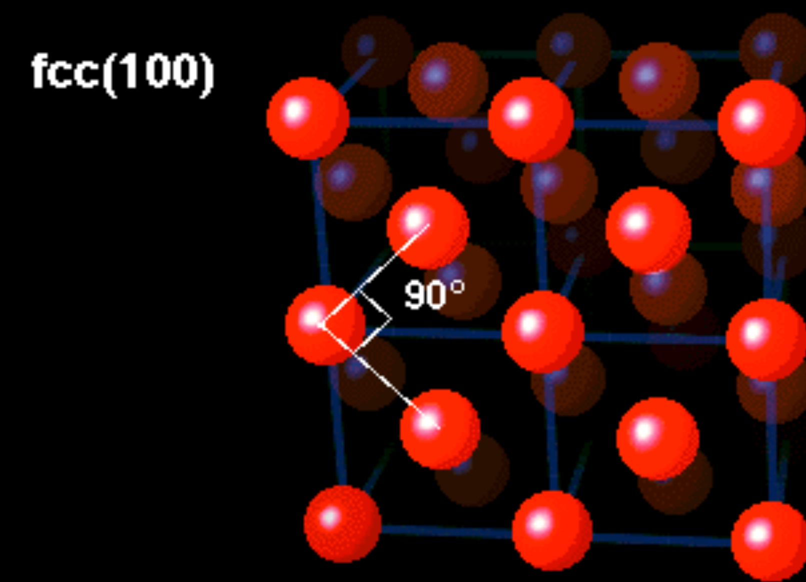


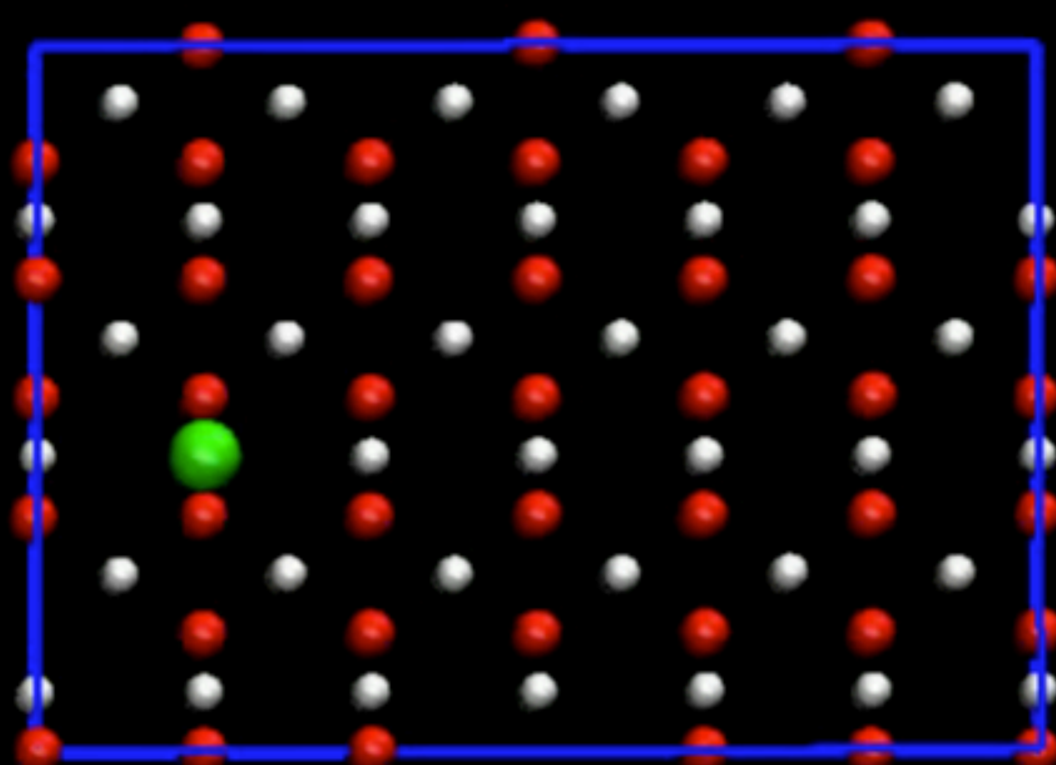


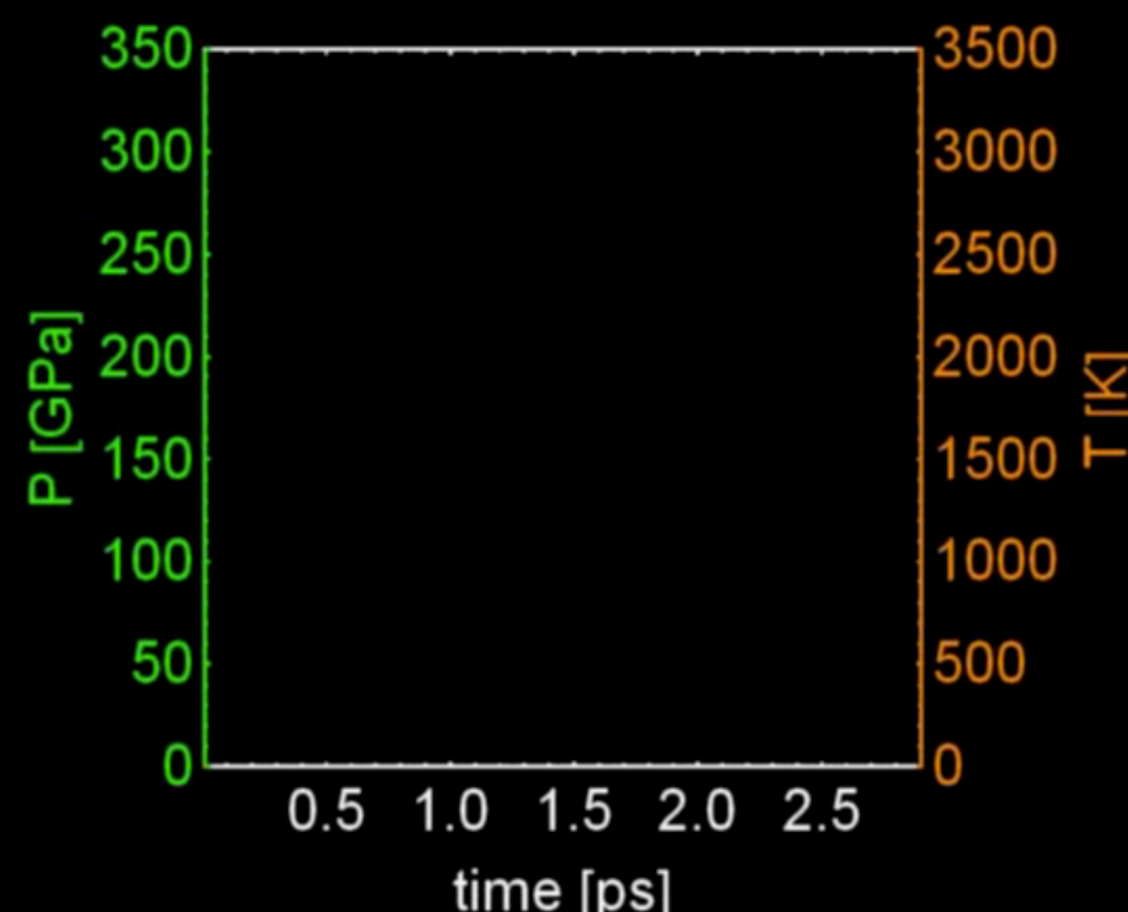


H_2O in Uranus



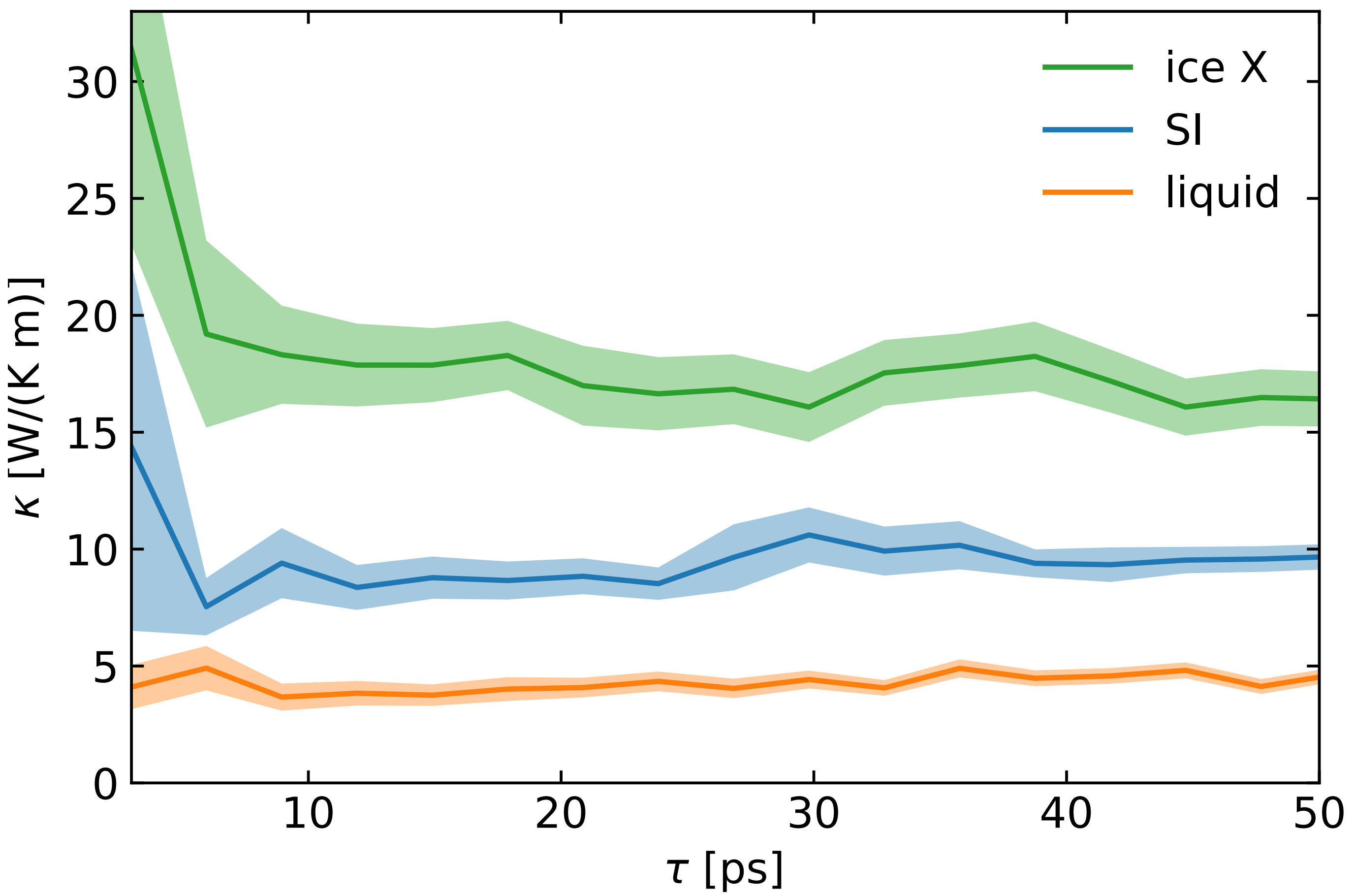




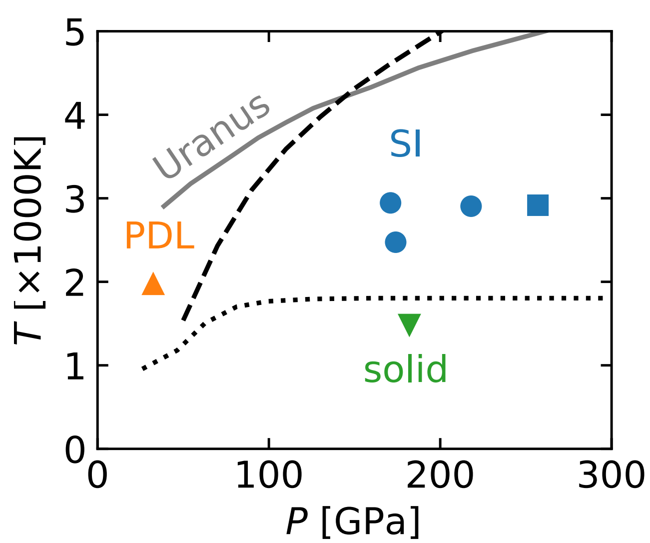


T = 3000 K P = 260 GPa

H_2O in Uranus



phase	κ [W/(Km)]	σ [S/cm]	$D_{H(O)}$ [$Å^2$/ps]	ρ [g/cm^3]	T [K]	P [GPa]
ice X ▼	16.1 ± 1.1	–	–	3.52	1488 ± 45	182 ± 1
SI^B ●	9.4 ± 0.6	135 ± 7	4.97 ± 0.05	3.39	2474 ± 78	174 ± 2
SI^B ●	10.7 ± 0.7	180 ± 5	7.44 ± 0.09	3.35	2945 ± 88	171 ± 2
SI^B ●	9.9 ± 0.7	198 ± 9	7.23 ± 0.07	3.61	2905 ± 86	218 ± 2
SI^F ■	12.8 ± 1.0	256 ± 8	7.26 ± 0.07	3.82	2917 ± 93	257 ± 2
PDL ▲	4.2 ± 0.3	45 ± 5	3.01 ± 0.04 0.92 ± 0.02	2.04	1970 ± 60	33 ± 1



from: F. Grasselli, L. Stixrude, and S. Baroni, in preparation

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thanks to:

Federico Grasselli, SISSA

Lars Stixrude, UCLA

these slides at
http://talks.baroni.me