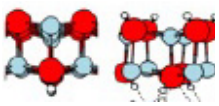

# Quantum transition: when deuterium breaks the symmetry

***Sodium hydroxide (NaOH), (NaOH), does not exhibit any phase transition at low temperatures. By replacing hydrogen with deuterium (D), a transition appears at 153K between two distinct crystal structures, with a strong expansion (>5%). At room temperature, the structures of NaOD and NaOH become very similar. This spectacular transition induced by a simple isotopic exchange was detected in 1985 and had never been explained: generally, in condensed matter, nuclei are considered classical objects (unlike electrons, naturally regarded as quantum). In this context, statistical properties are insensitive to isotopes. INSP researchers managed to elucidate this phenomenon, using a quantum description of the nuclei.***

The main correction due to quantum mechanics with respect to the classical vision of nuclei is the presence of zero point energy, an elementary quantum effect: because of Heisenberg's uncertainty principle, quantum particles are never completely at rest and explore the potential energy landscape, even in the absence of thermal agitation. In NaOH and NaOD, the OH or OD groups feel a potential with two minima corresponding to two possible orientations of the hydrogen bonds. In NaOH, the zero point energy is greater than the barrier which does not allow the system to localize in either of these two minima. Thus, hydrogen bonds do not form and the OH groups remain vertical (on the left in the figure). In quantum slang, NaOH is a quantum paraelectric because the resulting dipole is zero.

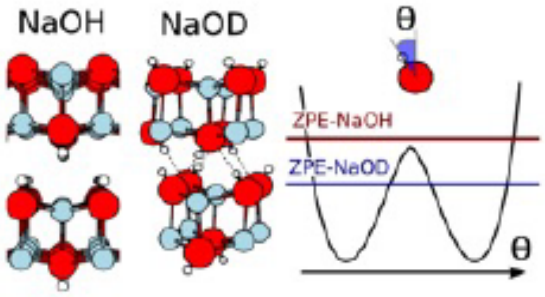


**Figure**
*The NaOH/D structure. In NaOH, quantum fluctuations prohibit the formation of hydrogen bonds and the OH groups oscillate around the vertical. Deuterium, although chemically equivalent, is heavier and therefore «less quantum». Its zero point energy (ZPE) is lower than the barrier, the OD groups are trapped in one of the potential wells and form hydrogen bonds which ensure the cohesion of the crystal... until thermal fluctuations take over!*

When D, heavier and «less quantum», replaces H, the zero point energy decreases below the height of the barrier and the OD groups are then trapped in one of the minima, the symmetry is broken towards an antiferroelectric order. As the temperature increases, OD tends to escape from the well, which breaks the hydrogen bonds and causes a sudden expansion at the transition temperature. At room temperature, NaOH and NaOD converge towards the same structure: this is the classical limit of quantum mechanics. The simulations also show that under pressure, hydrogen bonds are strengthened and symmetry is broken even in NaOH, which then behaves like NaOD.

The unexpected presence of a quantum transition in such a simple material and the competition between temperature and pressure effects opens a still largely unexplored field of research on quantum effects in the vast family of crystals whose cohesion is ensured by hydrogen bonds.

**Reference**
"When Quantum Fluctuations Meet Structural Instabilities: The Isotope- and Pressure-Induced Phase Transition in the Quantum Paraelectric NaOH"
**S. Schaack, E. Mangaud, E. Fallacara, S. Huppert, P. Depondt** and **F. Finocchi**
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