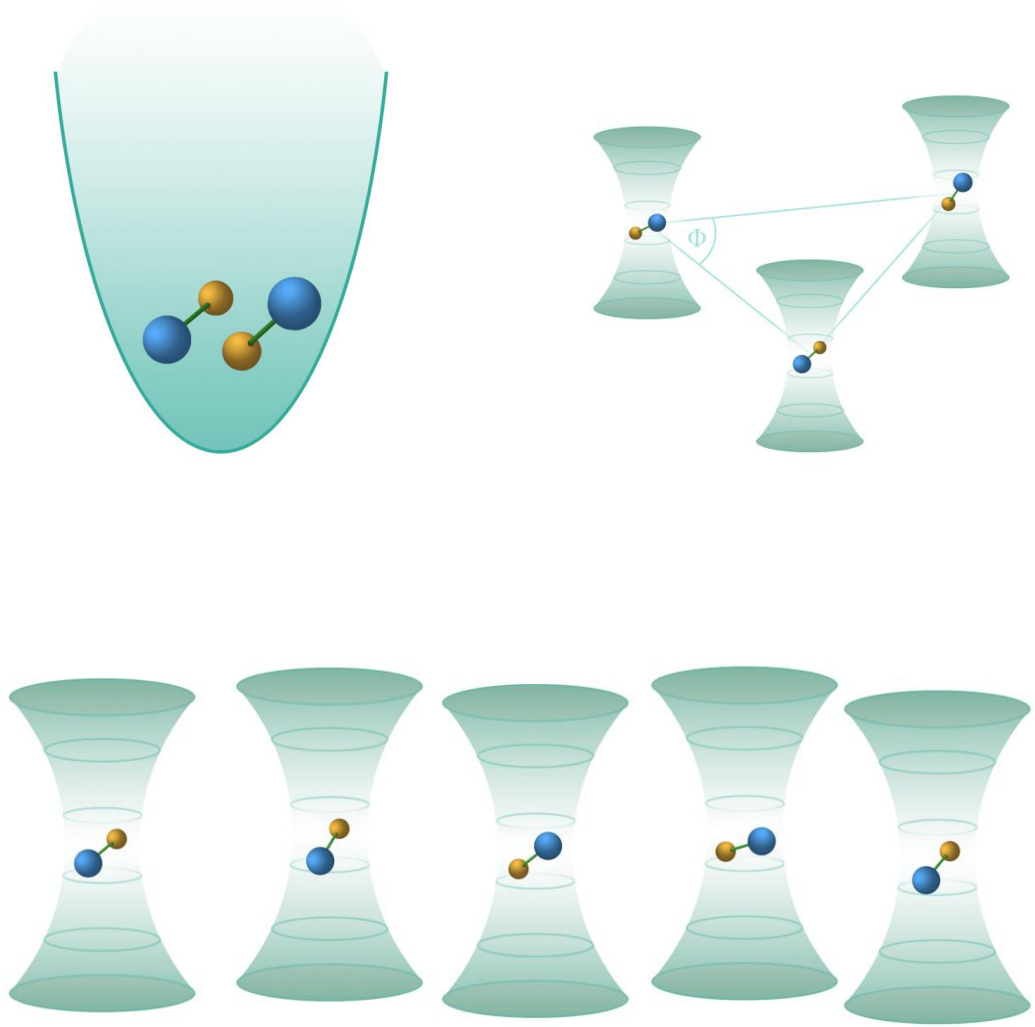
# Interplay of magnetic and electric properties of ultracold molecular systems

**Anna Dawid**

University of Warsaw
& ICFO, Barcelona

with Michał Tomza and Maciej Lewenstein



# Outline

Ultracold molecules:
state-of-the-art

Results – highlights:
how electric and magnetic properties of molecules are intertwined

Take-home messages

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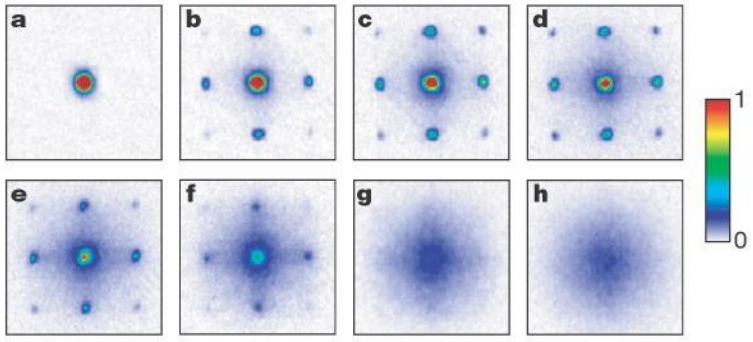
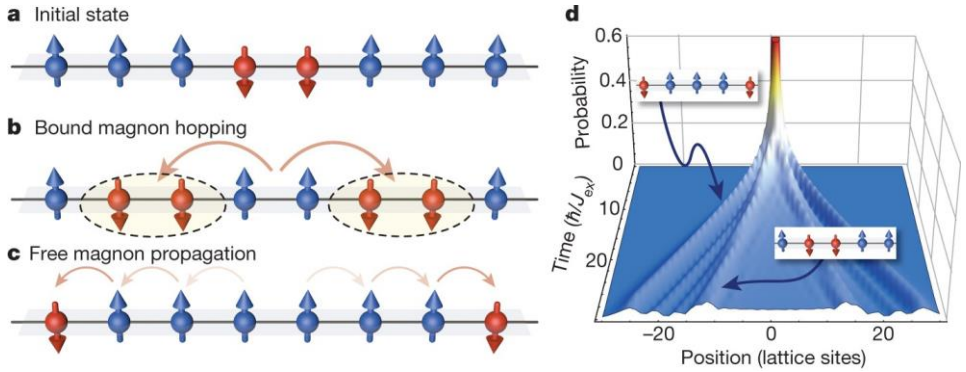
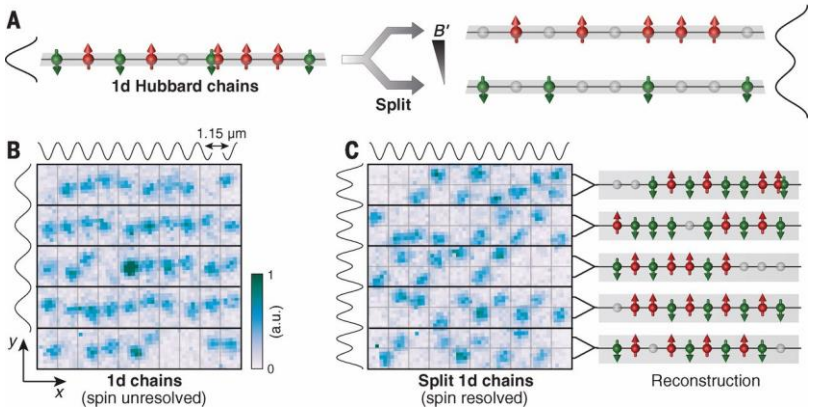
# Many-body physics with ultracold atoms



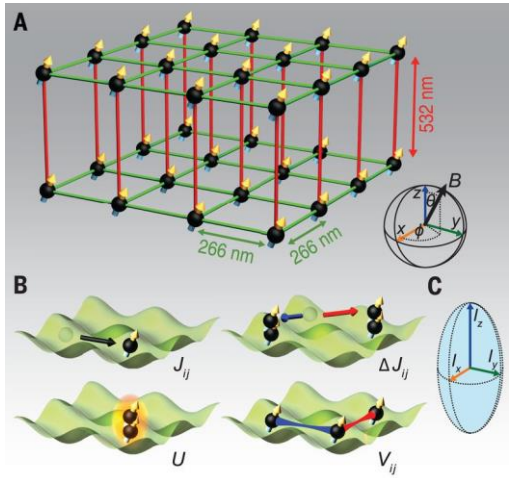

Greiner *et al*. Nature, 415, 2002



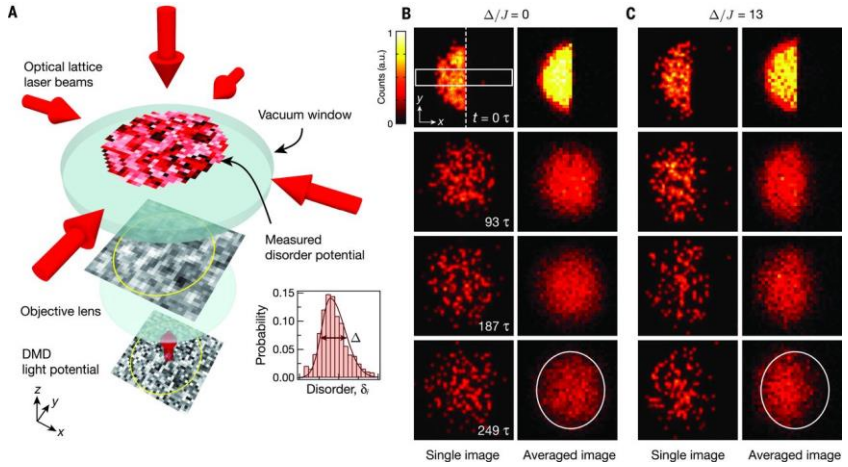

Fukuhara *et al*. Nature, 502, 2013




Boll *et al*. Science, 353, 2016




Baier *et al*. Science, 352, 2016

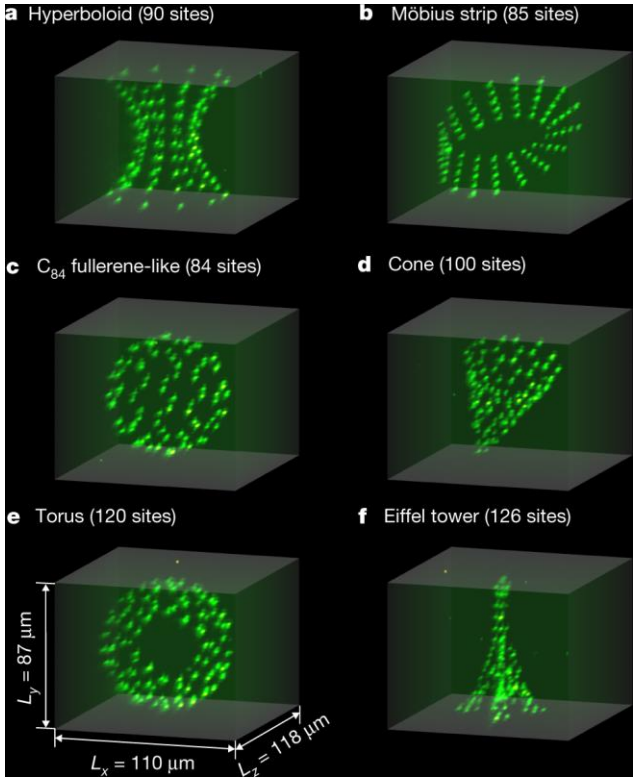


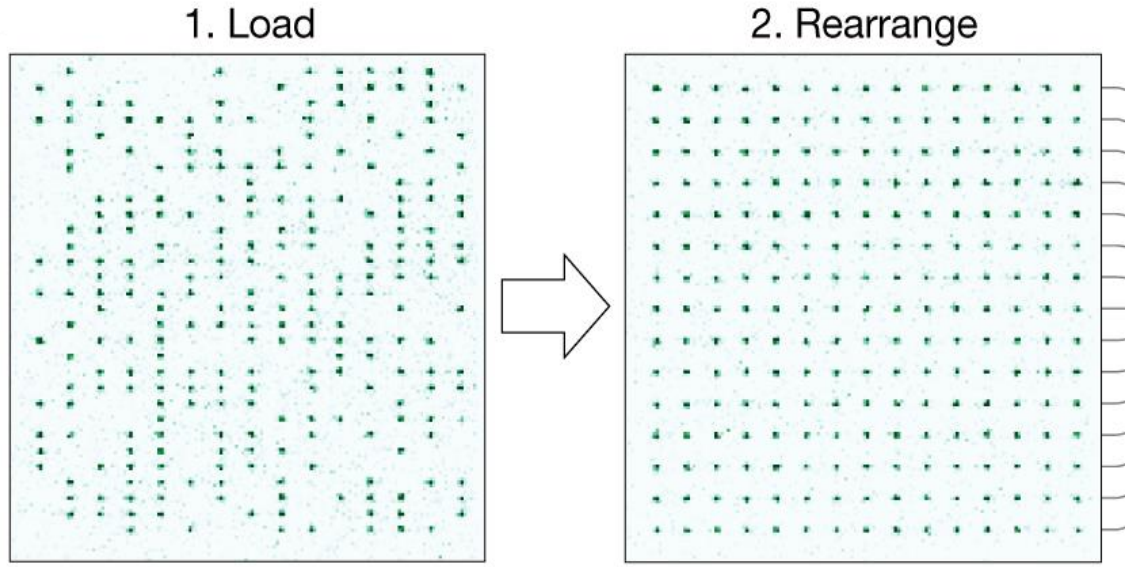

J. Choi *et al*. Science, 352, 2016

# Quantum control at a single-particle level

Science **354**, 1024 (2016)

Nature **561**, 79 (2018)



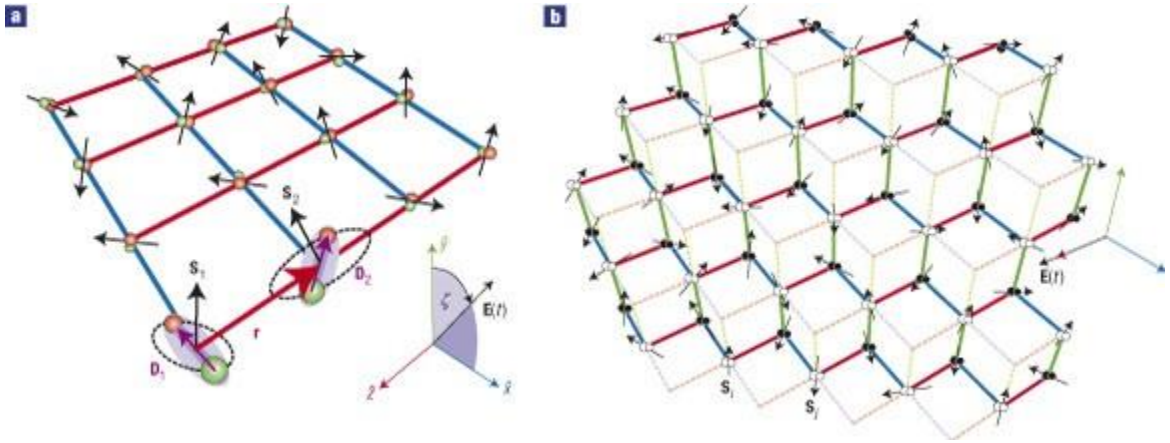

Nature **595**, 7866 (2021)

# Replacing atoms with molecules

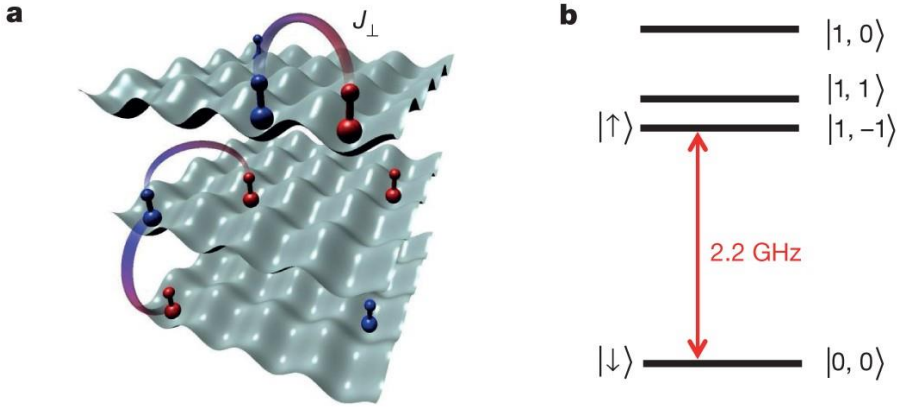
- Isotropic and short-range interactions
- Magnetic dipole moment
- Electronic structure, fine and hyperfine structure

- **Anisotropic** and **long-range** interactions
- Magnetic **+ electric dipole moment**
- Electronic, fine and hyperfine **+ rotational, vibrational structure**

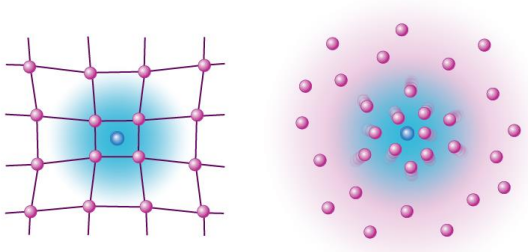
# Molecular promises



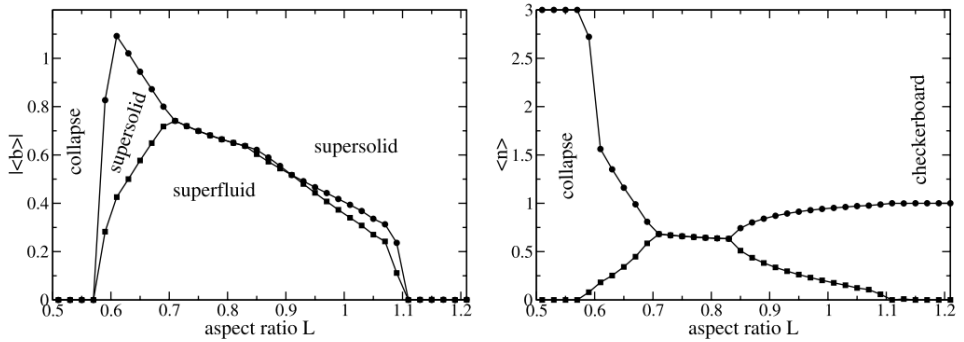

Micheli, Brennen, & Zoller. Nat. Phys., **2**, 341, 2006




Yan *et al.* Nature, **501**, 521, 2013



e.g. Herrera *et al.* Phys. Rev. Lett., **110**, 223002, 2013



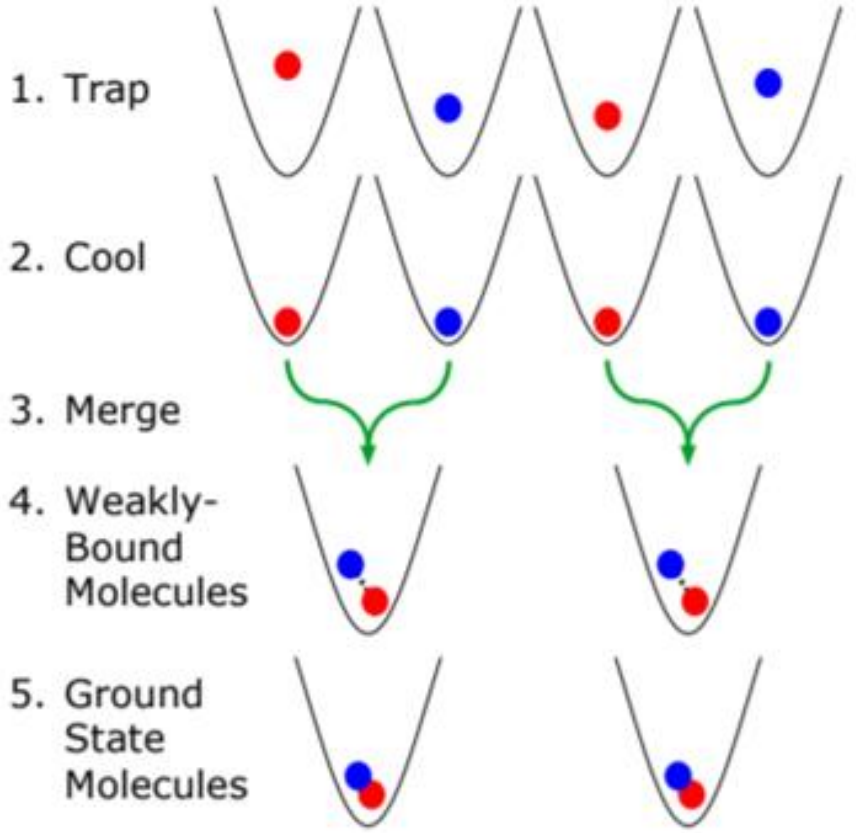

Góral, Santos & Lewenstein. Phys. Rev. Lett., **88**, 170406, 2002

# Towards full control over molecules

- Bottom-up approach

  Ni group: NaCs
  Wuhan group: RbRb

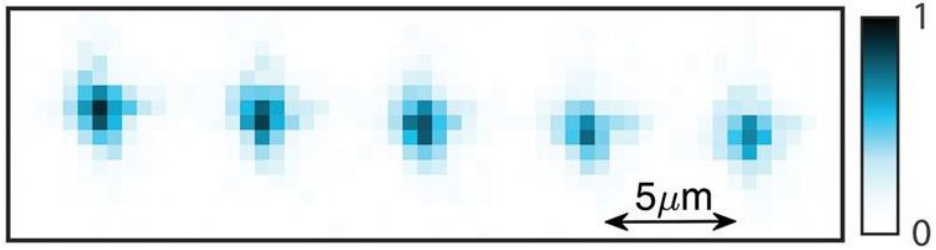
Science **360**, 900 (2018)
Science **370**, 331 (2020)



# Towards full control over molecules

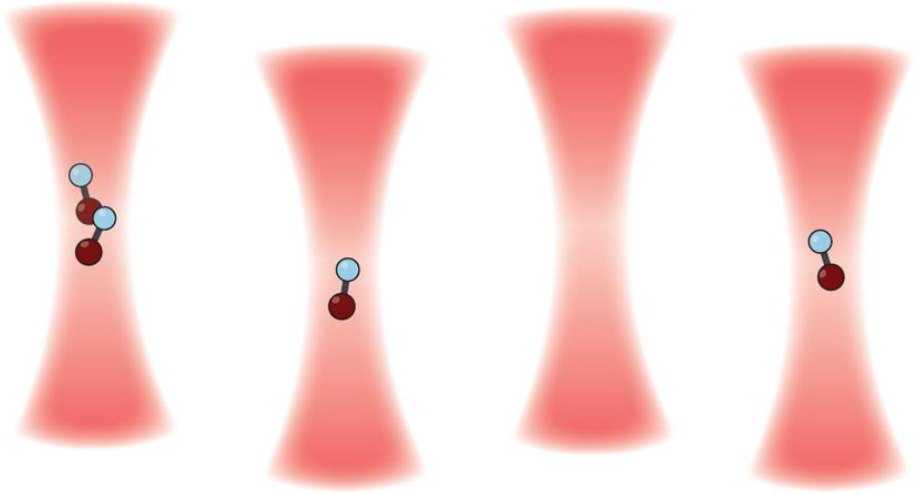
- Laser cooling of molecules, then loading to traps

Doyle/Ketterle/Ni: CaF

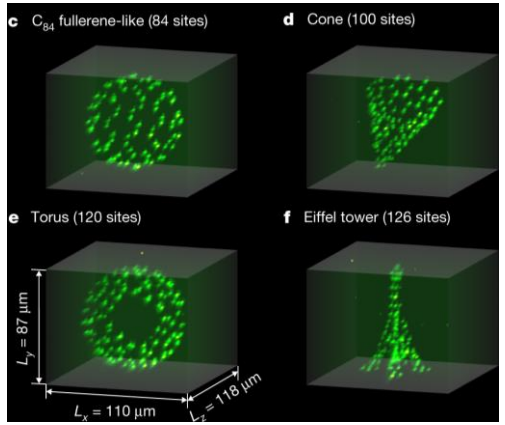



Phys. Rev. Lett. **119**, 103201 (2017)
Science **365**, 1156 (2019)

# Quantum control at a single-particle level



Science **365**, 1079 (2019)

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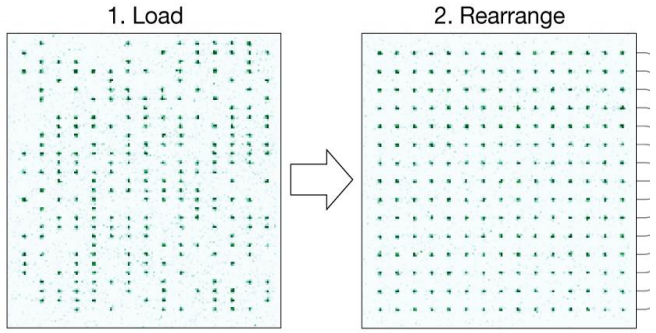



Nature **595**, 7866 (2021)

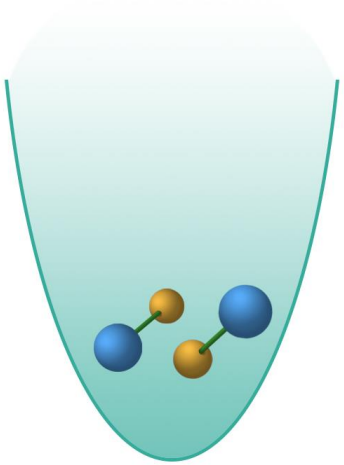
# Outline

Ultracold molecules:
state-of-the-art

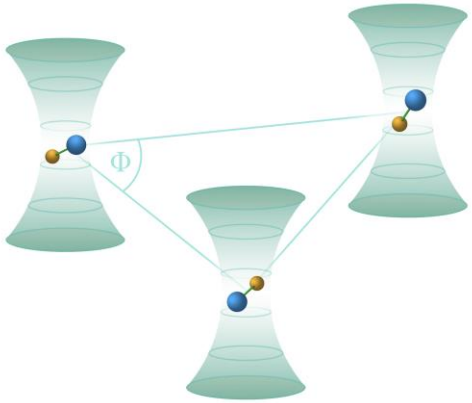
Results – highlights:
how electric and magnetic properties of molecules are intertwined

Take-home messages

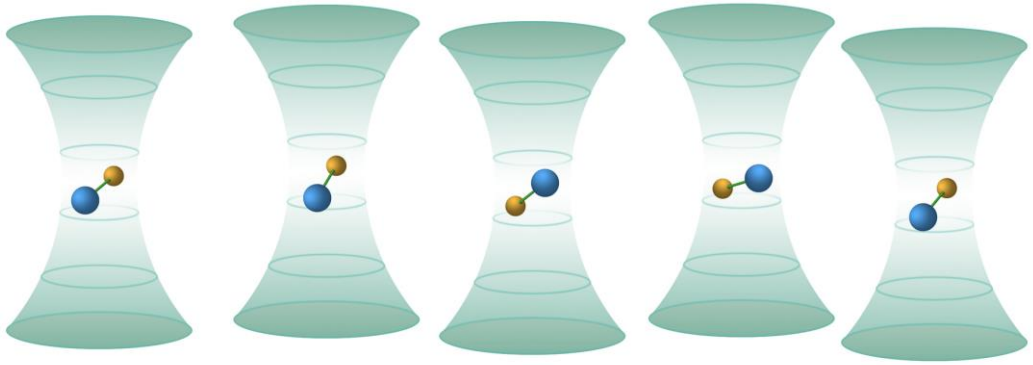
two molecules
in a 1D harmonic trap



few molecules
with controlled geometries

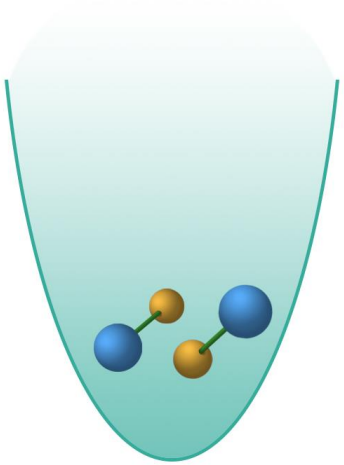



highly magnetic
and polar molecules



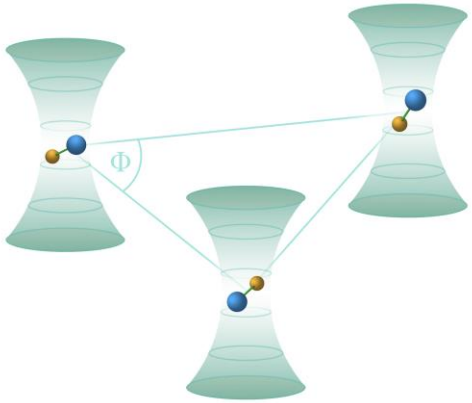
1D chain of molecules

**two molecules**
**in a 1D harmonic trap**



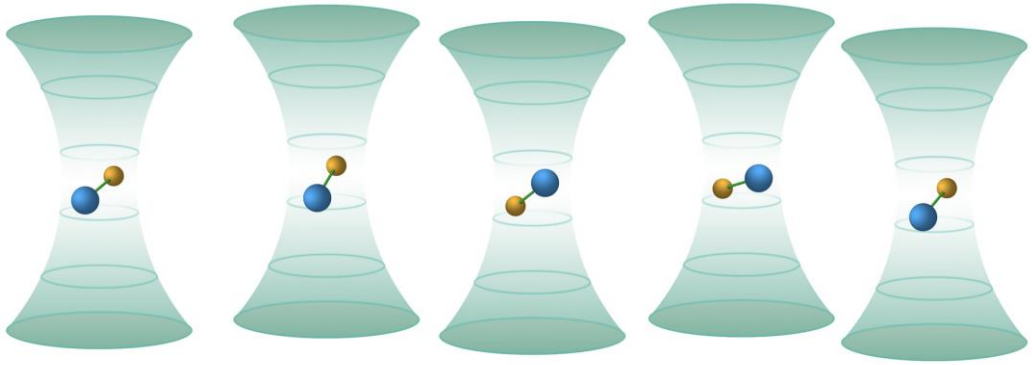
*prototypical example, on-site intermolecular interactions*

**few molecules**
**with controlled geometries**



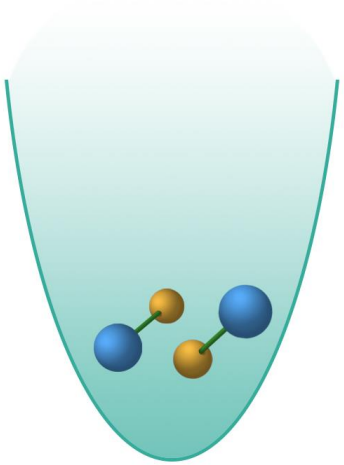

*interplay of "electric" and magnetic momenta, frustration?*

**highly magnetic and polar molecules**



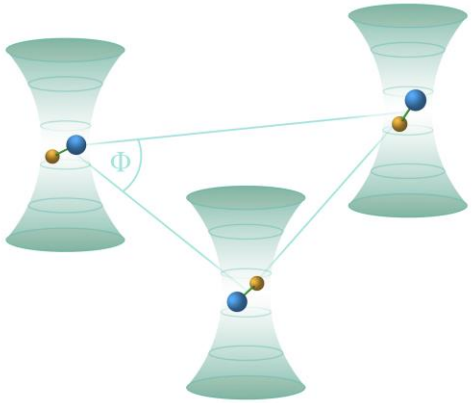
**1D chain of molecules**
*topological phases?*

**two molecules in a 1D harmonic trap**



*prototypical example, on-site intermolecular interactions*

**few molecules with controlled geometries**

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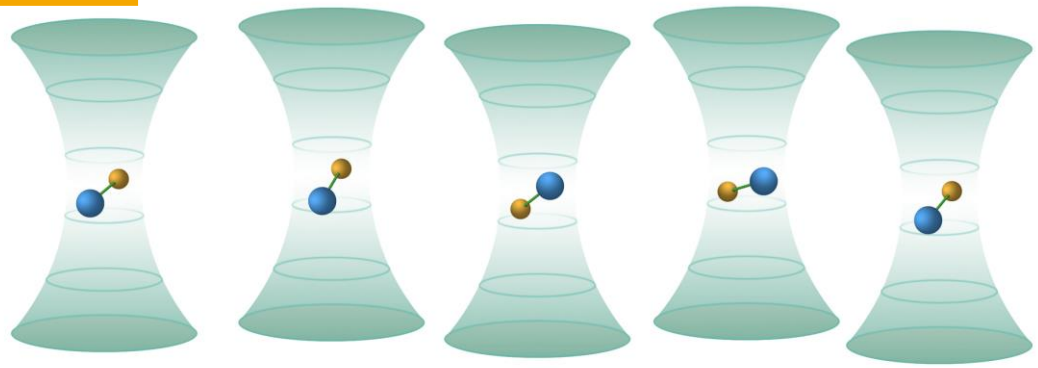

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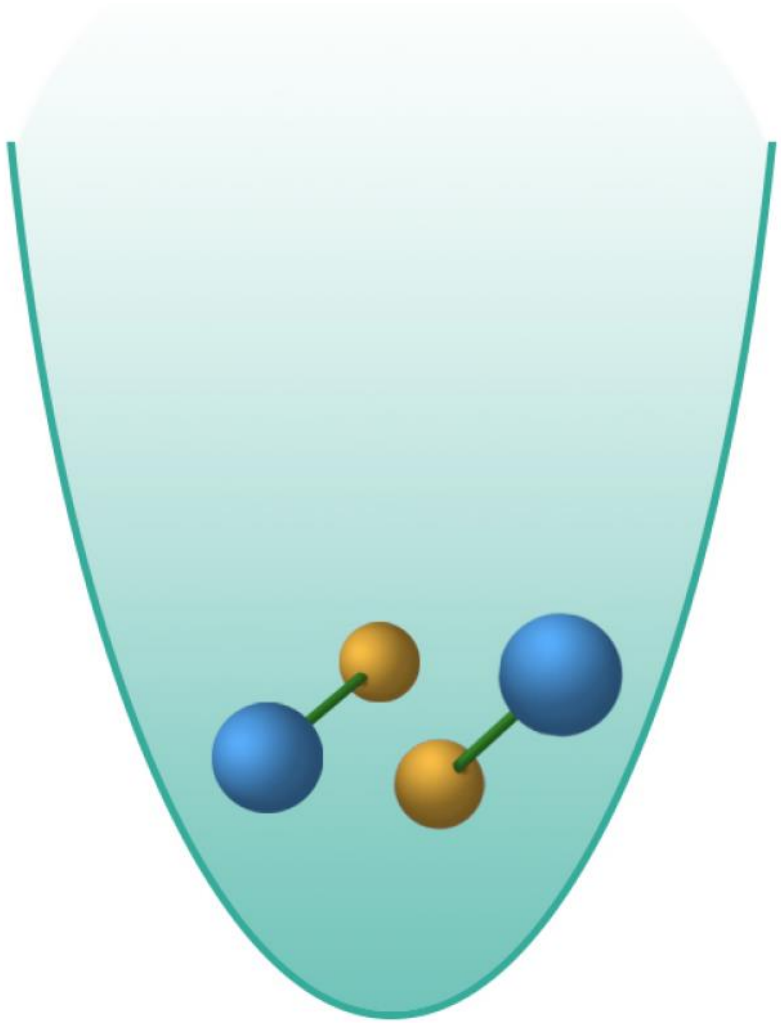
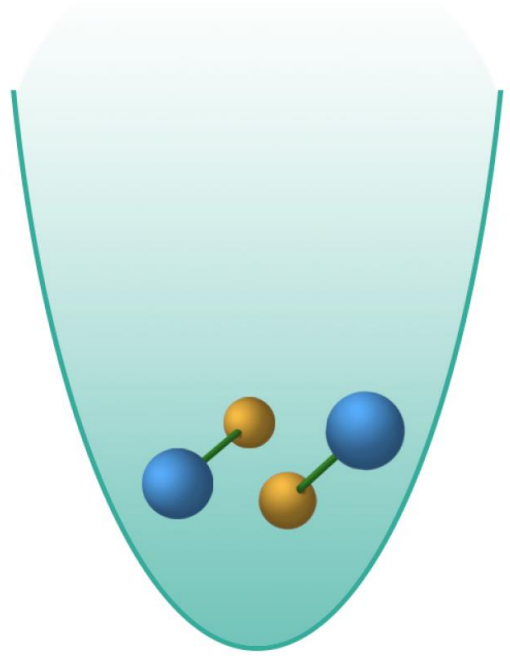


# Molecular model

- Harmonic trapping
- Molecules rotate as quantum rigid rotors
- Aniso- and isotropic interaction
- Electronic spin-rotation coupling
- External electric and magnetic field

# What's going on



anisotropic interaction

electric field

rotational structure

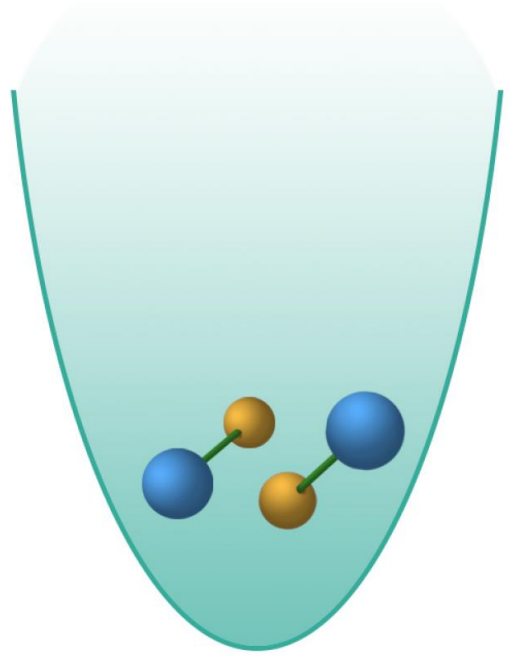
spin-rotation coupling

magnetization

*z*-projection of electronic spin

magnetic field

# What's going on



anisotropic interaction

electric field

rotational structure

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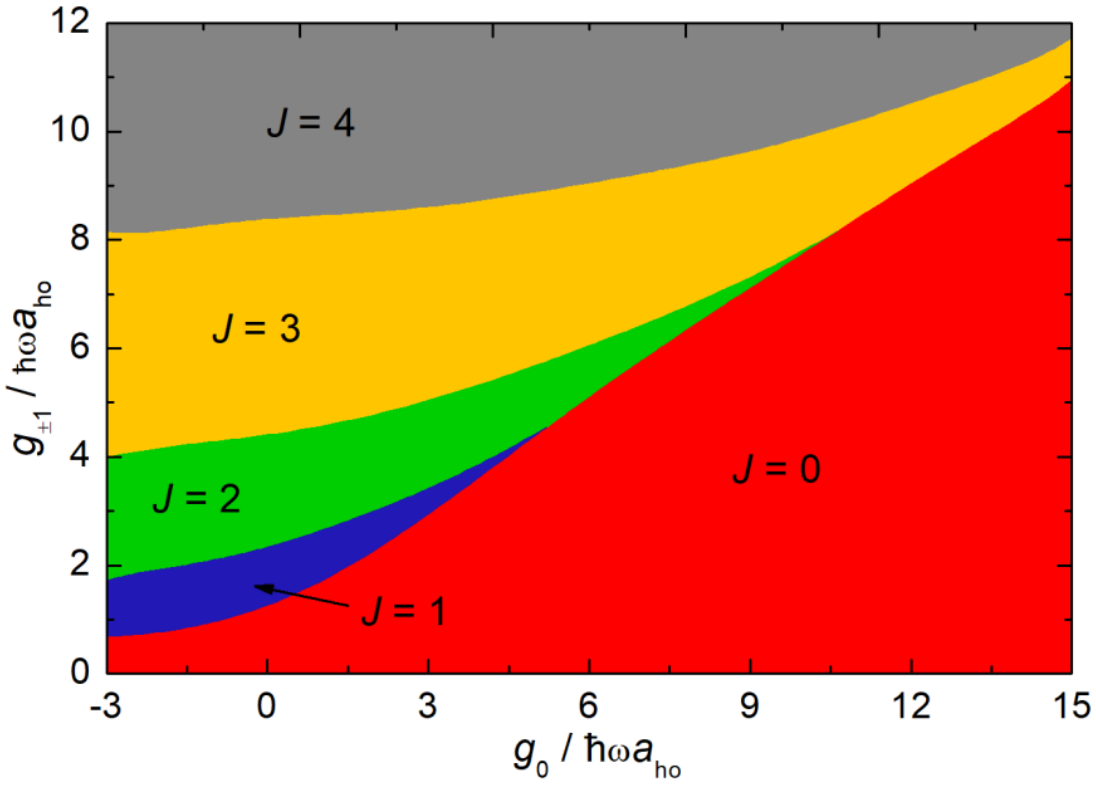
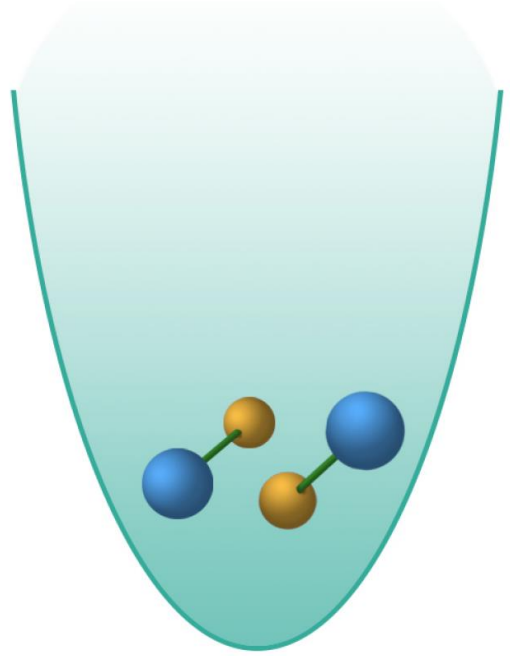
# Ground state with $J_{tot} \neq 0$!




Total rotational momentum
of the ground state
as a function of the isotropic ($g_0$)
and anisotropic ($g_{\pm 1}$)
interaction strength

Dawid et al., Phys. Rev. A **97**, 063618 (2018)

# What's going on



anisotropic interaction

electric field

rotational structure

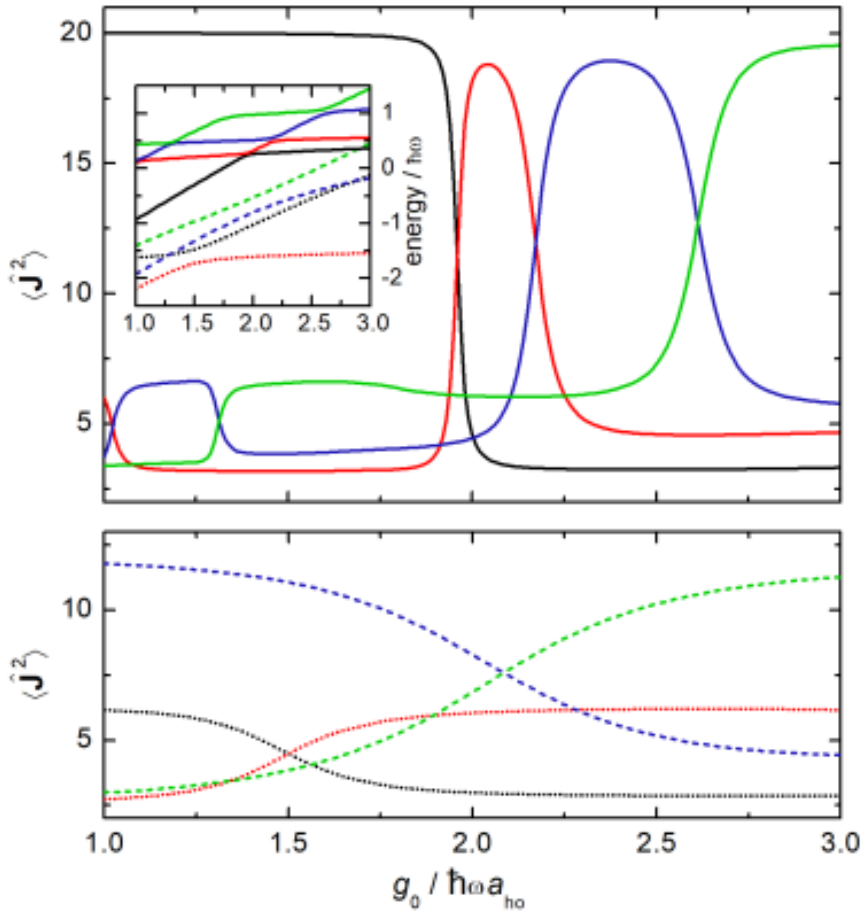
spin-rotation coupling

magnetization

*z*-projection of electronic spin

magnetic field

# Total rotational angular momentum can be pumped into the system with external electric field!

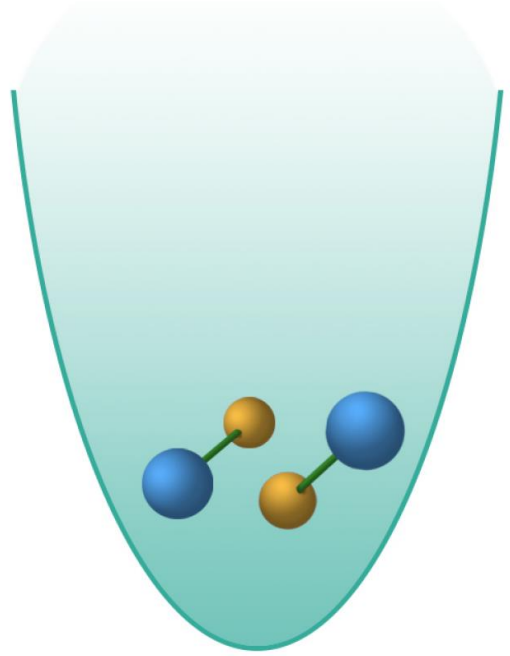



$$d\mathcal{E} = 2.5\,\hbar\omega$$

Mean values of the square of the total rotational angular momentum operator for selected eigenstates as a function of the isotropic ($g_0$) interaction strength

Dawid et al., Phys. Rev. A **97**, 063618 (2018)

# What's going on



anisotropic interaction

electric field

rotational structure

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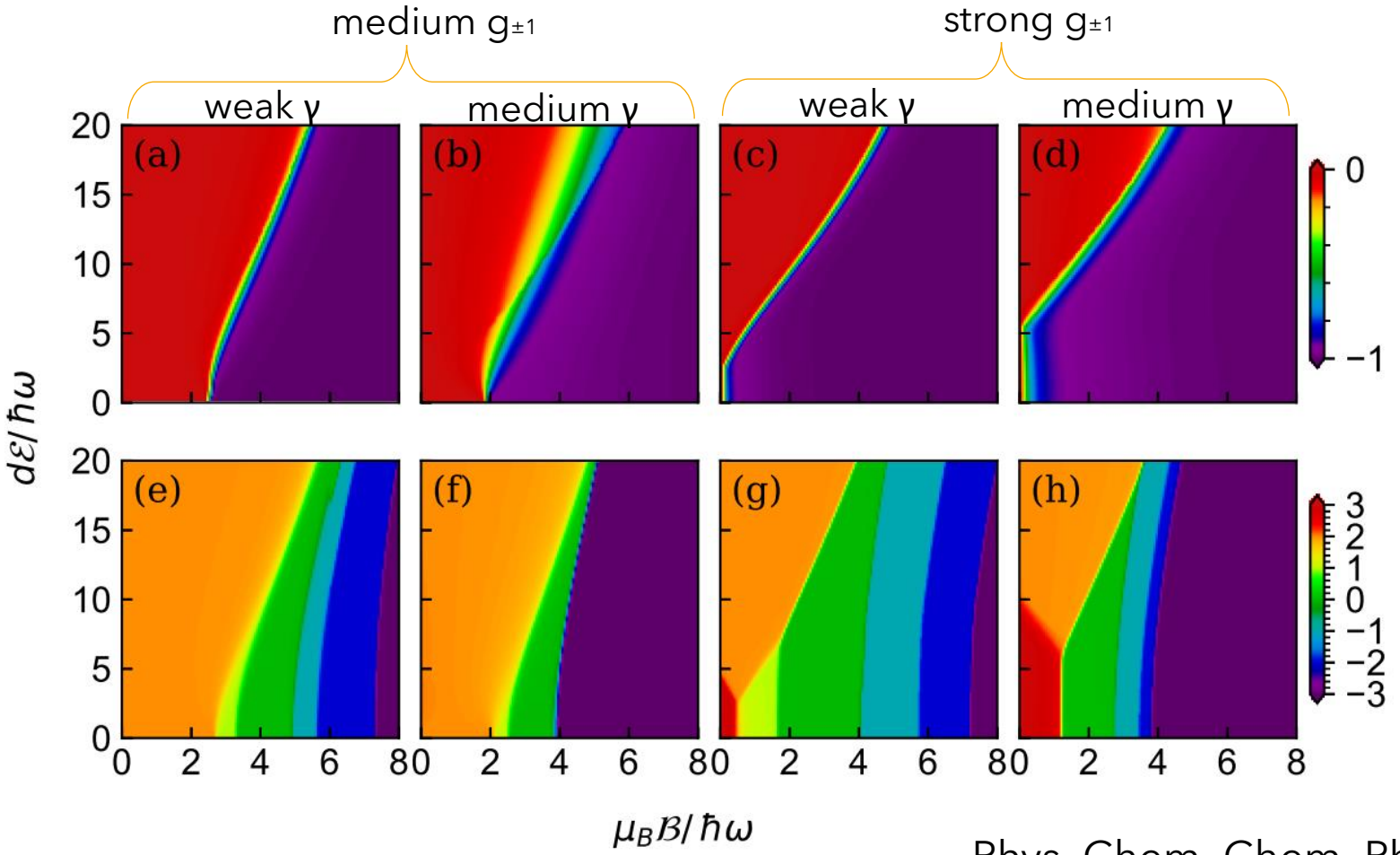
magnetic field

# Magnetization can be controlled with external fields!

Electric E vs. magnetic field B strength magnetization diagrams

spin 1/2
($M_{tot}$ = 0)

spin 3/2
($M_{tot}$ = 2)




**γ - spin-rotation coupling**

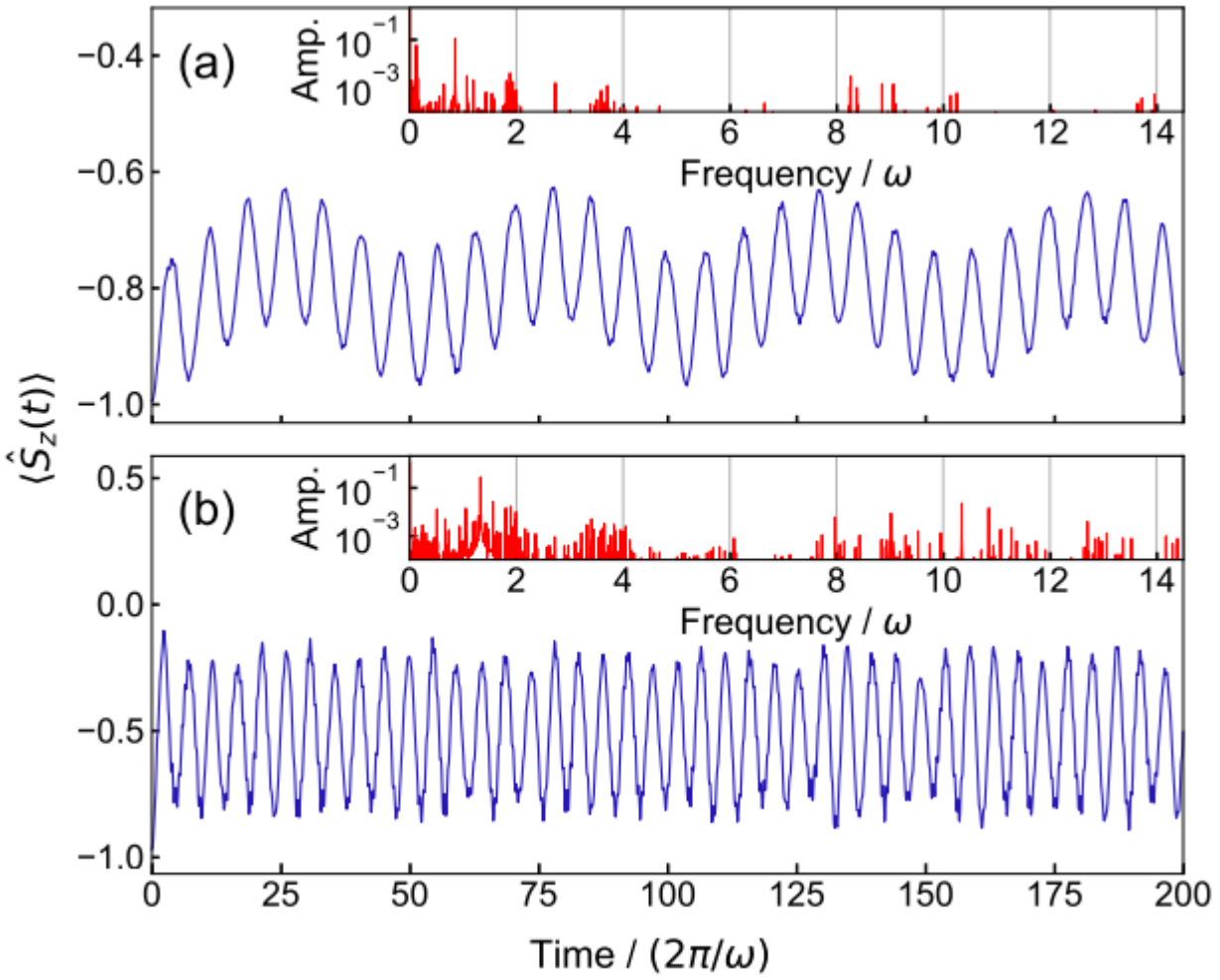
**$g_{\pm 1}$ – anisotropic interaction strength**

Dawid & Tomza,
Phys. Chem. Chem. Phys. **22**, 28140 (2020)

# Spin-rotation coupling:

**quench** of external **electric** field

**observable**:
*z*-projection of the **magnetic** spin angular momentum

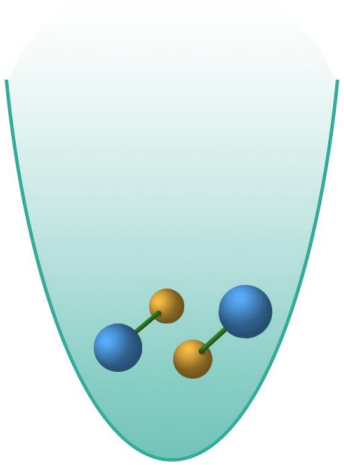



weak γ

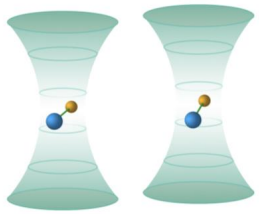
medium γ

Dawid & Tomza,
Phys. Chem. Chem. Phys. **22**, 28140 (2020)

**two molecules in a 1D harmonic trap**

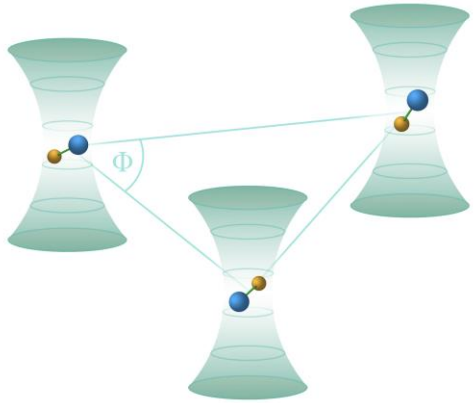


*prototypical example, intermolecular interactions*

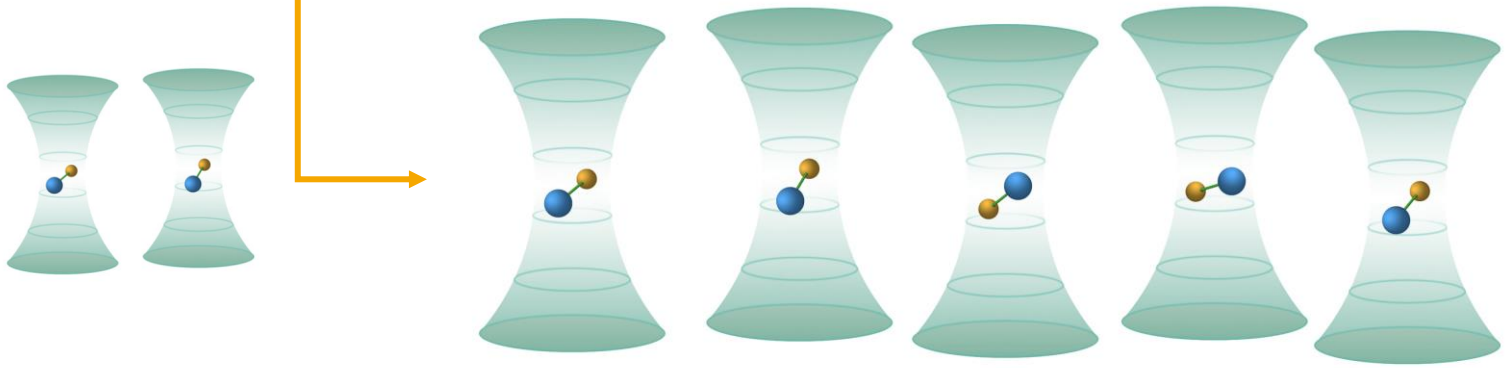


**highly magnetic and polar molecules**

**few molecules with controlled geometries**



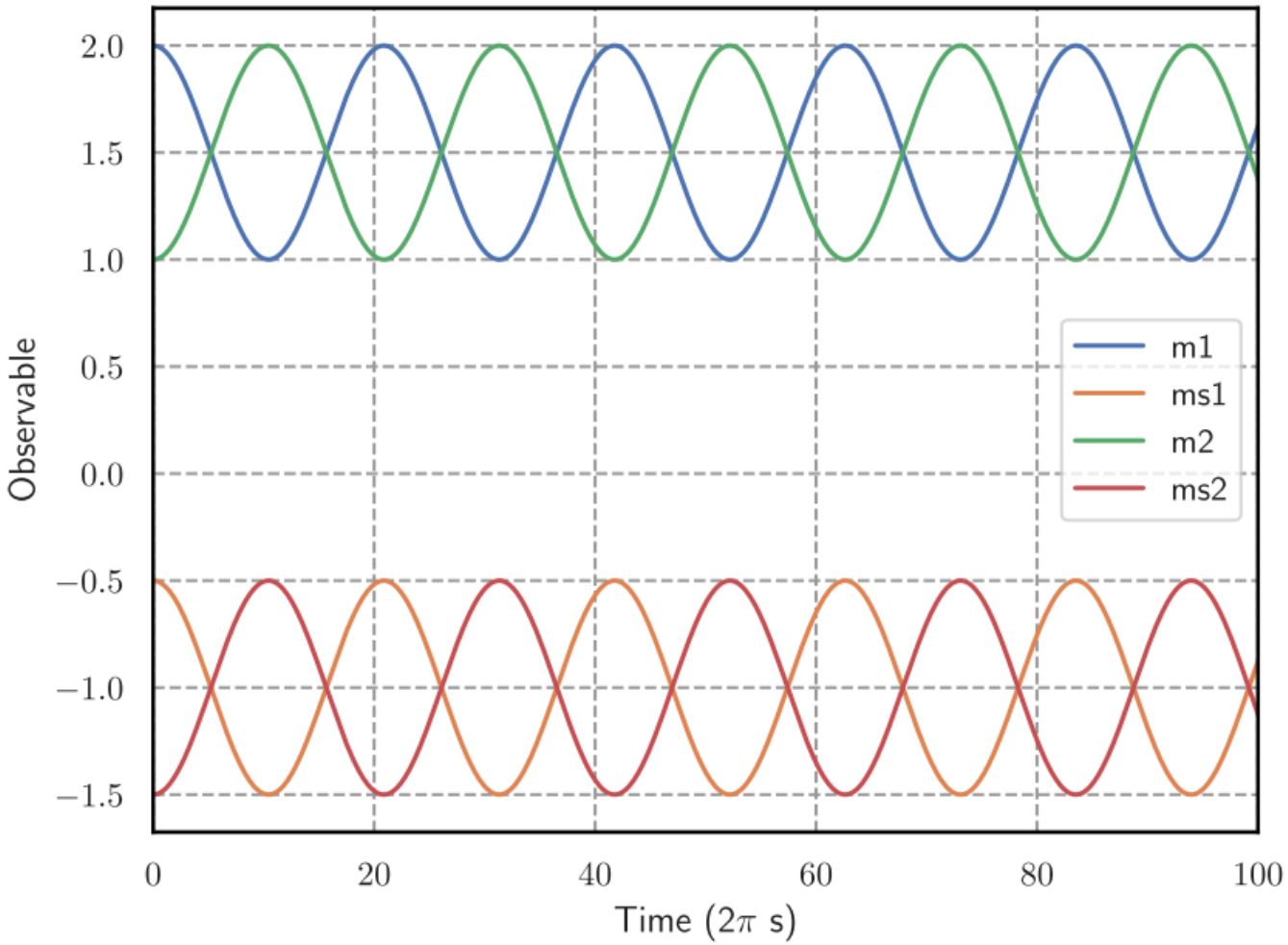

*interplay of "electric" and magnetic momenta, frustration?*



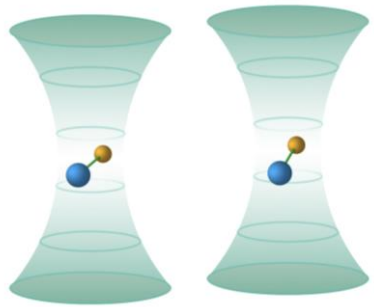
**1D chain of molecules**

*topological phases?*

preliminary!




# Two highly polar and magnetic molecules



# Outline

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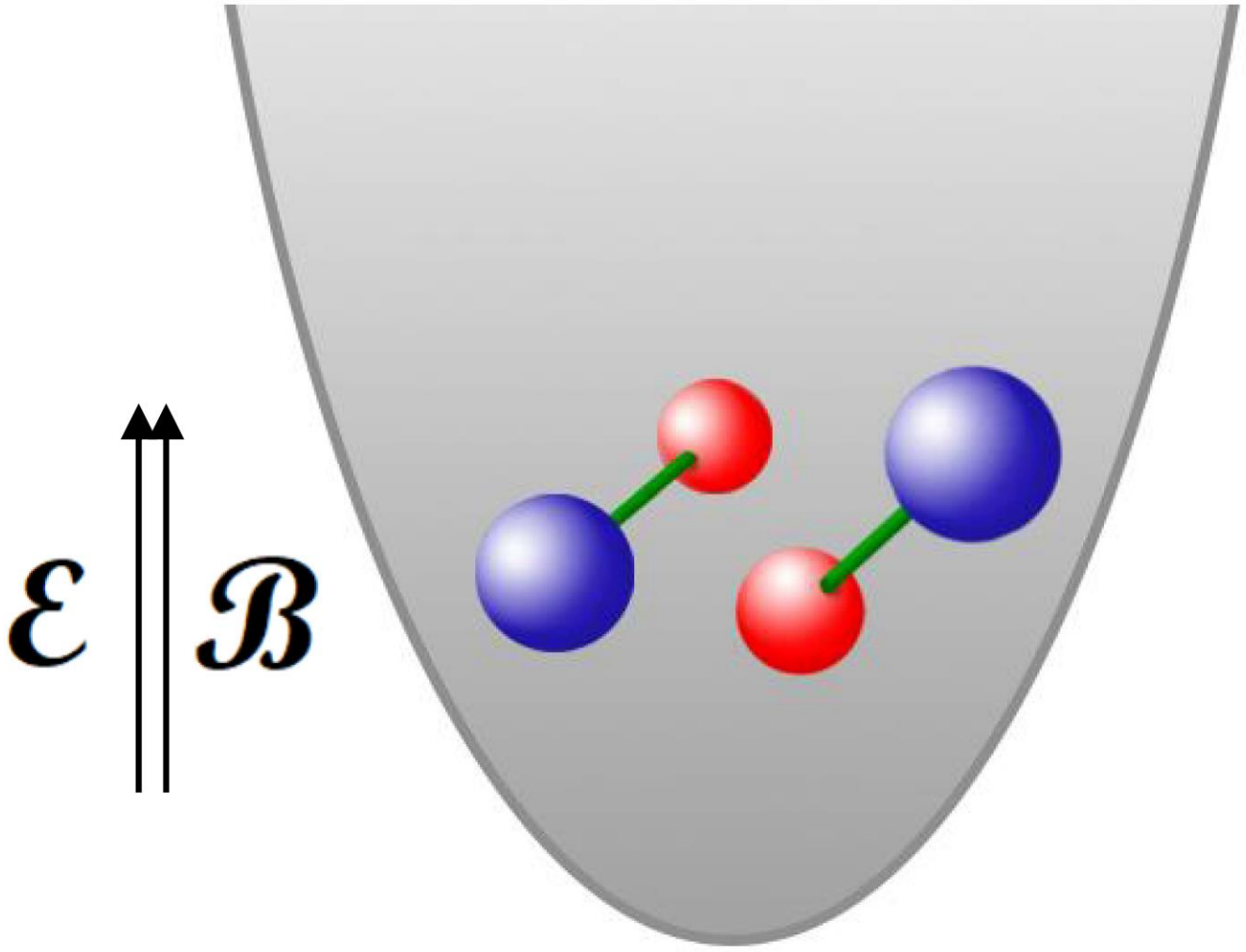
# Take-home messages

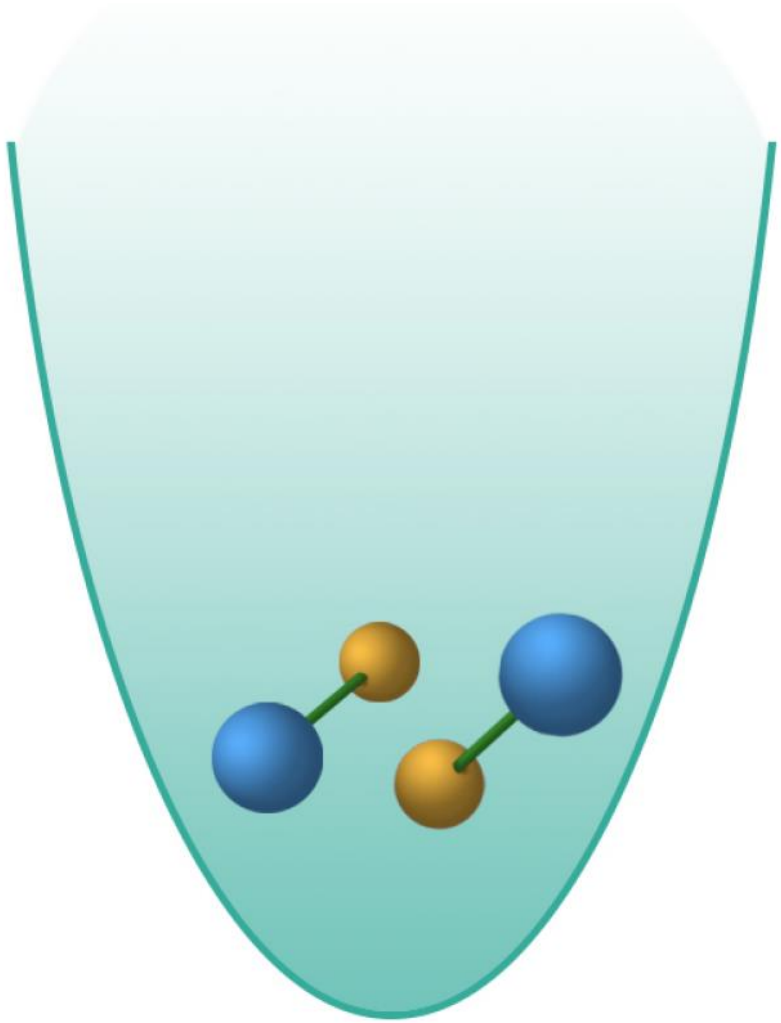
- Molecular electronic spin couples to the molecular rotation (~hundreds kHz)
- External electric field targets rotational structure, while magnetic field acts on spins
- We have a natural coupling of magnetic and electric properties in the molecules!




# Thank you for your attention!

Code available at: http://doi.org/10.5281/zenodo.3985911

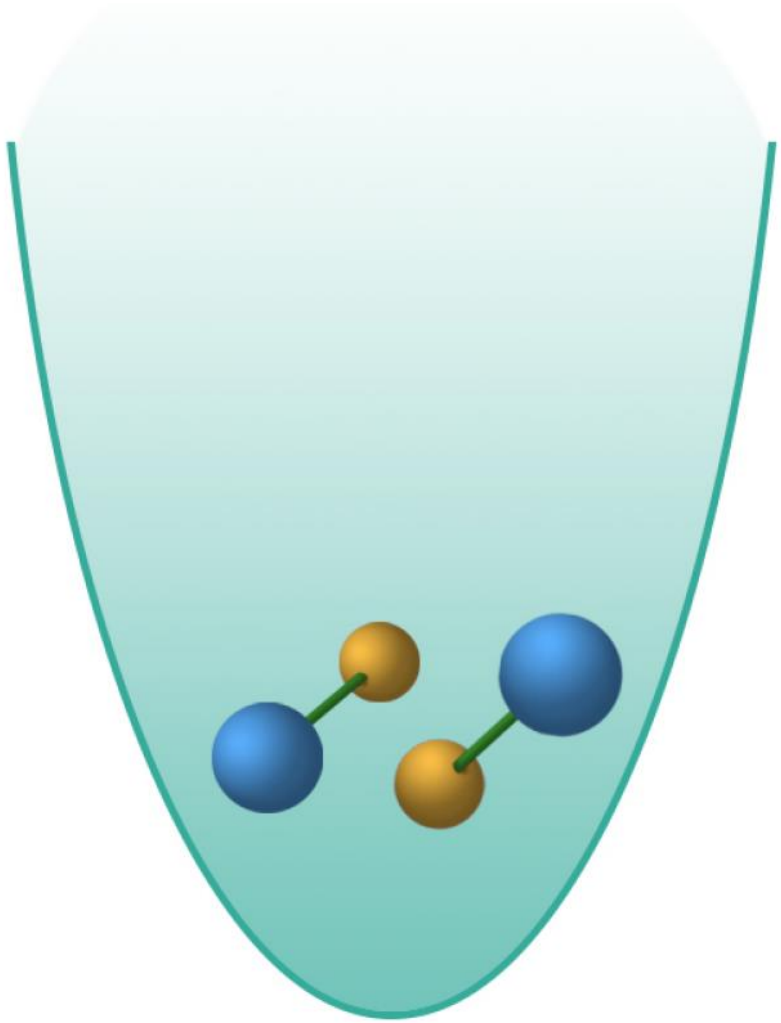
A. Dawid, M. Lewestein, M. Tomza. 2018. Phys. Rev. A **97**, 063618 (arXiv:1804.09168)
A. Dawid, M. Tomza. 2020. Phys. Chem. Chem. Phys. **22**, 28140-28153 (arXiv:2010.11899)



# Molecular model

$$\hat{H} = \hat{H}_{\text{trap}} + \hat{H}_{\text{mol}} + \hat{H}_{\text{field}} + \hat{H}_{\text{int}}$$

$$\hat{H}_{\text{trap}} = \sum_{i=1}^{2} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{2} \frac{1}{2} m\omega z_i^2$$

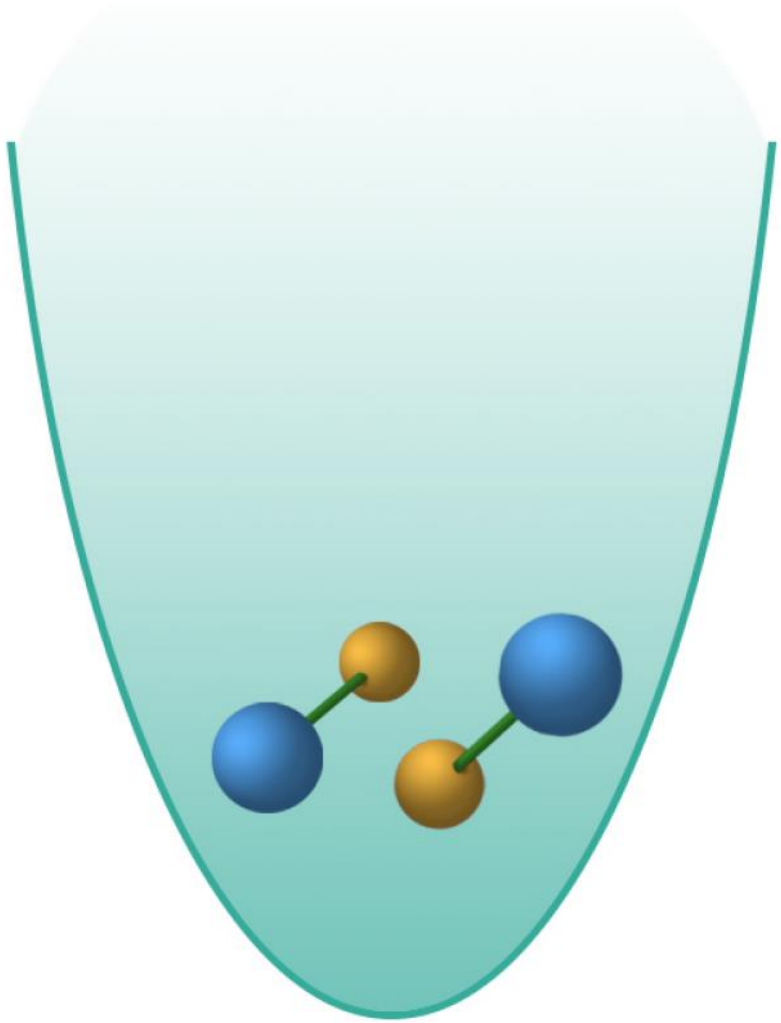


# Molecular model

$$\hat{H} = \hat{H}_{\text{trap}} + \hat{H}_{\text{mol}} + \hat{H}_{\text{field}} + \hat{H}_{\text{int}}$$

$$\hat{H}_{\text{rot}} = \sum_{i=1}^{2} B\,\hat{\mathbf{j}}_i^2\,,$$

$$\hat{H}_{\text{spin-rot}} = \sum_{i=1}^{2} \gamma\,\hat{\mathbf{s}}_i \cdot \hat{\mathbf{j}}_i\,,$$

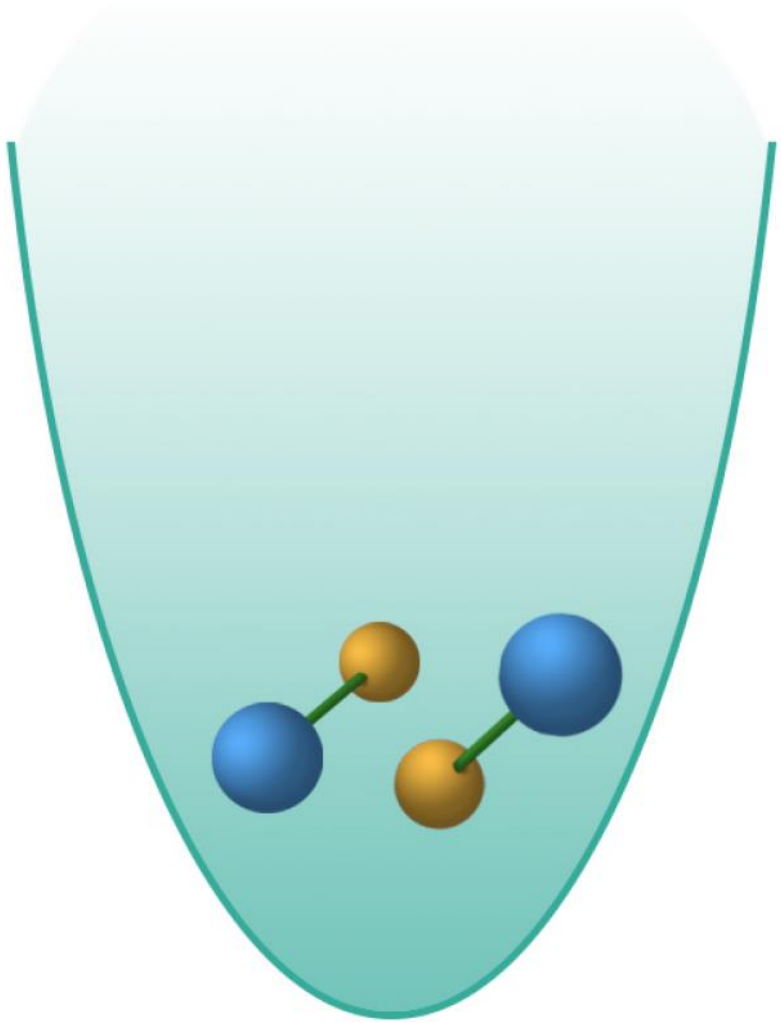


# Molecular model

$$\hat{H} = \hat{H}_{\text{trap}} + \hat{H}_{\text{mol}} + \hat{H}_{\text{field}} + \hat{H}_{\text{int}}$$

$$\hat{H}_{\text{Stark}} = -\sum_{i=1}^{2} \hat{\mathbf{d}}_i \cdot \mathcal{E}\,,$$

$$\hat{H}_{\text{Zeeman}} = 2\mu_B \sum_{i=1}^{2} \hat{\mathbf{s}}_i \cdot \mathcal{B}$$



# Molecular model

$$\hat{H} = \hat{H}_{\text{trap}} + \hat{H}_{\text{mol}} + \hat{H}_{\text{field}} + \hat{H}_{\text{int}}$$

$$\hat{H}_{\text{iso}} = \sum_{\alpha} g_0 \delta(z_1 - z_2) \hat{P}_0 \,,$$

$$\hat{H}_{\text{aniso}} = \sum_{\alpha \neq \alpha'} g_{\pm 1} \delta(z_1 - z_2) \hat{P}_{\pm 1}$$

$$\text{with } \hat{P}_0 = |J, M, j_1, j_2\rangle \langle J, M, j_1, j_2|$$

$$\hat{P}_{\pm 1} = |J, M, j_1 \pm 1, j_2\rangle \langle J, M, j_1, j_2 \mp 1| + \text{H.c.}$$