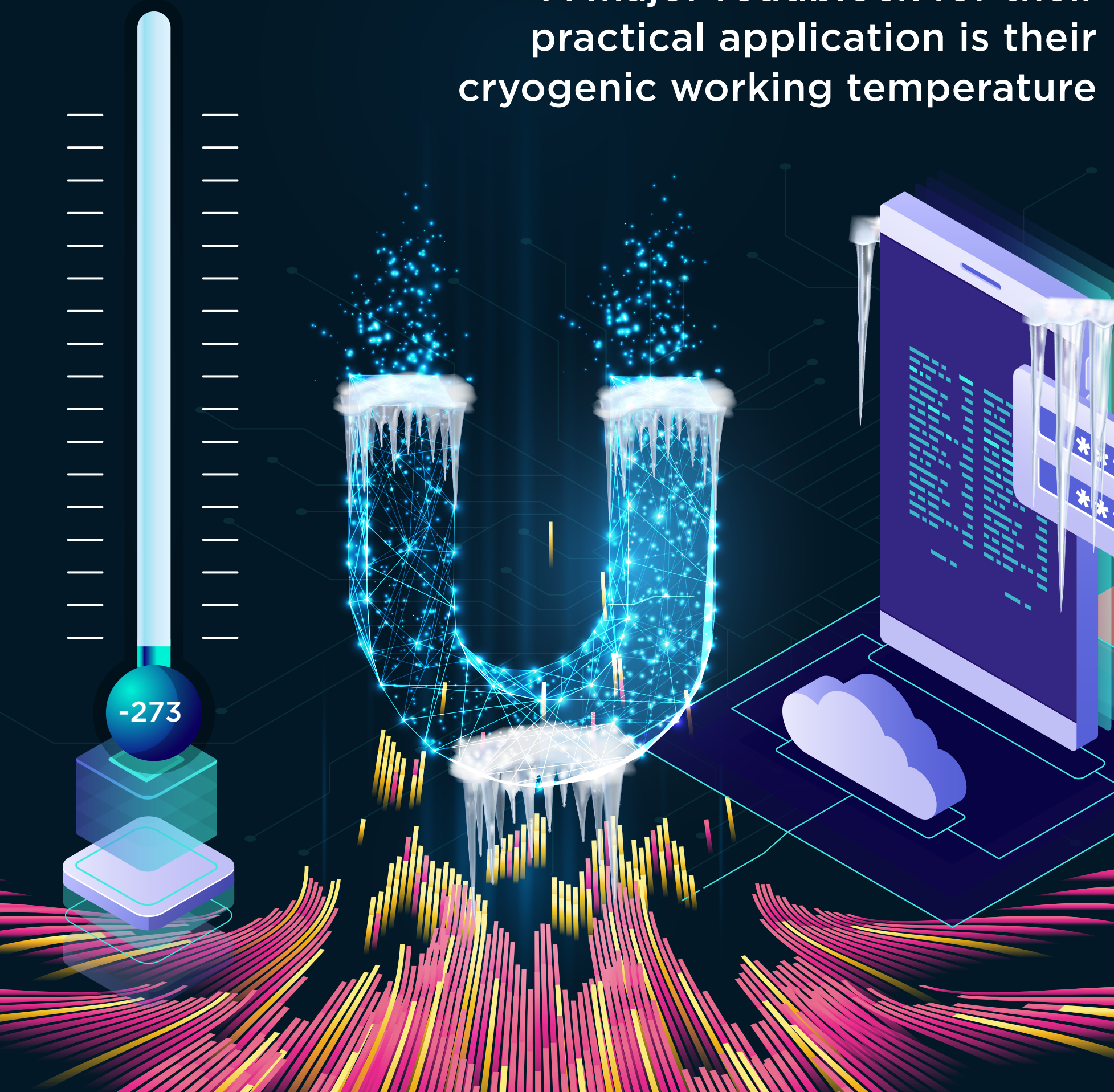


Efficient design of High-temperature Single-molecule Magnets

Single-molecule magnets (SMMs) represent the limit of miniaturization and are attractive potential candidates for information storage

A major roadblock for their practical application is their cryogenic working temperature



An efficient methodology to explore and chemically design new SMMs with higher operating temperatures

First-principles approach to simulate spin relaxation in f-block SMMs



Just one Complete Active Space Self Consistent Field calculation

Faster than state-of-the-art methods

Accurate and practical

Thermal dependence of relaxation pathways

Theoretical tools reported could be used to design and predict the behaviour of SMMs that can function at higher temperatures

Chemical
Science



Design of high-temperature f-block molecular nanomagnets through the control of vibration-induced spin relaxation

Baldoví *et al.* (2019) | DOI: 10.1039/C9SC03133B

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