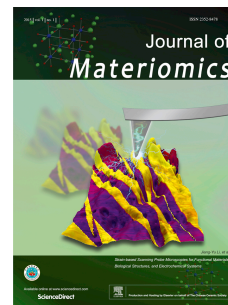


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Quantitative structure-property relationship study of cathode volume changes in lithium ion batteries using ab-initio and partial least squares analysis

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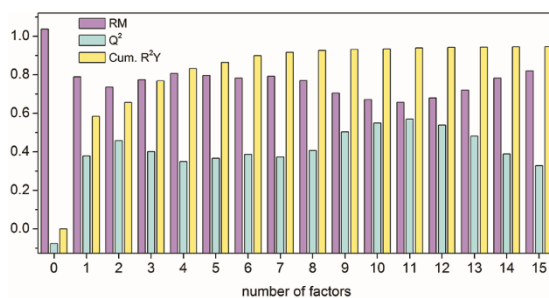
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Graphical Abstract:**Highlights:**

Building the PLS modelling on QSAR formulation of cathode volume change in LIBs based on ab-initio calculation data;

Investigating the factors related to the volume change within 28 oxide cathodes including with spinel- and layered-structure;

Assigning the variables those make major contributions to the volume change during delithiation;

Exhibiting the promising future of the virtual screening and combinatorial design of low-strain cathode materials for LIBs.

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