We introduce a methodology to disentangle the role of electronic ($\Delta N$) and lattice degrees of freedom ($Q$) in phase transitions, solving this long-standing issue. We find the role of a linear electron-lattice coupling to be key.

$$F(\Delta N, Q) = \frac{k Q^2}{2} - \frac{1}{2}g Q \Delta N + F_{el}(\Delta N)$$

Provided $k$, $g$ and $\Delta N(Q)$ are known, one can then obtain $F_{el}(\Delta N)$ and $\Delta F(\Delta N, Q)$ by integration of equation of state. 

Here we use DFT+DMFT for the ES calculation.

Electronic (left panel) and total energy (central panel) as functions of octahedral breathing mode amplitude ($Q$), and electronic disproportionation ($\Delta N$).

Energy vs orbital polarization $\Delta N$ for thin film $\text{Ca}_2\text{RuO}_4$ for different strains. Tensile strain favors an insulating state/higher MIT temperature.

As $F_{el}(\Delta N) > 0$, $kQ^2 > 0$, the electron-lattice coupling $-\frac{1}{2}g Q \Delta N$ is key to driving the transition.

This methodology can be applied to any electronic phase transition. One simply needs:

1) A method to perform electronic structure calculations (DFT, DFT+U, DFT+DMFT, DFT+HF)
2) A well-defined electronic ($\Delta N$) degree of freedom.
3) A well-defined lattice degree ($Q$) of freedom.
4) A methodology to extract and define $g$ and $k$.

Further References:
2) OE Peil et al, PRB, 99, 2019
3) AB. Georgescu et al, PNAS, 29, 2019
4) Q. Han, AJ Millis, PRL, 121, 067601, 2018