

Abstract Submitted  
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**A DFT investigation of pressure effects in the infinite-layer  $ACuO_2$  cuprate superconductor for  $A=\{Mg, Ca, Sr, Ba\}$**  BEN MALLET, NICOLA GASTON, JAMES STOREY, GRANT WILLIAMS, ALAN KAISER, JEFFERY TALLON, MacDiarmid Institute — We use density functional theory to investigate external-pressure and “internal-pressure” effects in the infinite-layer cuprate  $ACuO_2$  for  $A=\{Mg, Ca, Sr, Ba\}$ , where internal-pressure is induced by ion-size substitution. Where these materials have been synthesised we find good agreement between our calculated structural parameters and the experimental ones. We find that these non-hydrostatic pressure-effects can have a significant effect on the superconducting energy gap via modifications to the electronic dispersion. Furthermore, pressure alters the dispersion independently of how it is applied (internal or external) so that the superconducting energy gap correlates with the unit-cell volume.

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