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Organic Single Crystal ThermoChromic Materials

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The above titled project has focused on developing a combinatorial library of thermoChromic materials based on a naphthalene diimide (NDI) core functionalized with alkyl phenoxy substituents. The central thrust of the project was to expand our understanding of thermoChromic processes that we had observed in a phenylbutoxy-NDI system. Curiously, in our examination, we uncovered both thermoChromism and a thermosaliency. The latter property being a sudden kinetic release of energy upon heating. We were able to discern that this thermosaliency could be attributed to a change in crystal packing at a defined transition temperature, and this sudden change could be controlled to conduct physical work. In our first publication, (M. Dharmarwardana, R. P. Welch, S. Kwon, V. K. Nguyen, G. T. McCandless, M. A. Omary, J. J. Gassensmith *Chem. Commun.* **2017**, 53, 9890–9893) we fully described this system and we were able to demonstrate that single crystals of phenylbutoxy-NDI could lift metal weights over 100 times heavier than themselves.

Following that initial report, we began a systematic study of substitutions on the phenoxy group. Our results indicated that both the thermoChromism and thermosaliency were a general property of this class of molecules. We believe we have discovered a first “general class” of thermosalient materials in our phenoxy substituted NDI with the proviso that changing the substituent also changed the temperature at which the crystals underwent their phase transition and concomitant thermosalient effects. We also discovered we could control the temperature range of the thermoChromism in these derivatives, with some derivatives showing changes in color from red to yellow as temperatures increased and some derivatives showing the inverse—a change from yellow to red. As a proof-of-principle we were able to create polymer-crystalline blends and 3D print thermoChromic plastic sensors, which changed color upon exposure to different temperatures. These results were published in a special issue of *CrystEngComm* dedicated to rising young talent and is available on-line (M. Dharmarwardana, B. S. Arimilli, M. A. Luzuriaga, S. Kwon, H. Lee, G. A. Appuhamillage, G. T. McCandless, R. A. Smaldone, J. J. Gassensmith *CrystEngComm* **2018**)