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Turning liquid active ingredients into crystals

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We present a systematic way to embed liquid or volatile molecules inside crystalline materials in order to tune tuning their delivery for medicine or agrochemistry. Liquid or volatile formulations of active pharmaceutical ingredients (APIs) are intrinsically less stable and durable than solid forms. In fact most drugs and agrochemicals are manufactured and distributed as crystalline materials, and their action involves the delivery of the active molecule by a solubilization process either in the body or on the environment. The poor solubility of API or the reverse too high solubility of agrochemicals are problems often encountered in their formulation since these phenomena limit respectively the bioavailability of the API or the duration of the action of the agrochemical. However some important compounds for the human health or for the environment are liquid at room temperature; examples are thymol, eugenol, carvacrol, nicotine, propofol, and we present a twofold approach to embed them in crystalline hosts: by cocrystals and by MOFs. The formation of co-crystals alters solubility of solid phases, and is widely investigated for pharmaceuticals, agrochemicals, pigments, dyestuffs, foods, and explosives. In spite of this extremely high interest towards co-crystallization as a tool to alter solubility, practically no emphasis has been paid to using it as a means to stabilize volatile or labile or liquid products. In this work we trap and stabilize volatile and liquid APIs and agrochemicals in crystalline matrices by engineering suitable co-crystals. These new materials alter the physic state of the active ingredients allowing to expand the phase space accessible to manufacturing and delivery. We also explore the possibility to include liquid APIs inside the pores of suitable designed MOFs (Figure), again with the aim of stabilizing their solid state formulation.

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