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Self-assembling smart microscopic reagents to pioneer pourable electronics – turning chemistry inside-out?

First place in an EU competitive call on “Unconventional Computing”¹ was awarded to a collaborative proposal coordinated by Professor John McCaskill from the Faculty of Chemistry and Biochemistry. The project MICREAgents (EU contribution 3.4 M€) plans to build autonomous self-assembling electronic microreagents that are almost as small as cells. They will exchange chemical and electronic information to jointly direct complex chemical reactions and analyses in the solutions they are poured into. Four participating research groups at RUB (G. von Kiedrowski *Bioorganic Chemistry*, J. S. McCaskill *Microsystems Chemistry and BioIT*, J. Oehm *Analog Integrated Circuits* and P. Mayr *Integrated Digital Circuits*) from two faculties will join forces with top teams from across Europe, and from Israel and New Zealand to tackle this ambitious goal. The project heralds a major step beyond Lab-on-a-Chip devices towards the integration of chemistry and information technology.

John von Neumann envisioned information devices that can construct more complex machines than themselves, in his theory of self-reproducing automata², but he did not arrive at a robust architecture for this. Modern initiatives towards Living Technology, exploiting the core properties of living systems to push back this frontier, have been spearheaded by RUB in the past decade. McCaskill cofounded (2004-5) the European Centre for Living Technology in Venice (ECLT), an ongoing multi-university institution of which RUB is a member. He has also helped to link up a world-wide community on Sustainable Personal Living Technology (2010). This initiative requires a fundamental integration of molecular construction and information processing and thereby of chemistry and ICT (information and communication technology). Currently, RUB is assembling a roadmap in an EU coordination action (COBRA) for the area of chem-bio ICT, and indeed this integration is most developed in biological organisms. The MICREAgents project represents the next major research program towards these overarching initiatives, one that could change the level of fine-grained algorithmic control in chemical construction, bringing the important social goal of sustainable personal fabrication one step closer.

In order to create this programmable microscale electronic chemistry, MICREAgents (Microscopic Chemically Reactive Electronic Agents) will contain electronic circuits on 3D microchips (called **lablets**, diameter $\leq 100 \mu\text{m}$) that self-assemble in pairs or like dominos to enclose transient reaction compartments, using the electronics to control chemical access, surface coatings and reactions via physical and chemical processes such as electroosmosis, electrowetting and electrochemistry. Chemicals can be selectively concentrated, processed and released into the surrounding solution, under local electronic control, in a similar way to which the genetic information in cells controls local chemical

¹ European Union FP7 Future Emerging Technologies Program (Call 8)

² J. von Neumann in “Self-reproducing automata” edited and completed by A.W. Burks Univ. Illinois Press, Urbana and London (1966).

processes. The reversible pairwise association in solution of electronic surfaces in the nanometer range will also be used to avoid the prohibitive energetic costs of broadcast communication, allowing lablets to transfer information (including heritable information) from one to another. The *lablet* devices will integrate transistors, supercapacitors, energy transducers, sensors and actuators, involving electronically constructed nanofilms, and will be essentially genetically encoded, translating electronic signals into constructive chemical processing and recording the results of this processing. Instead of making chemical reactors to contain chemicals, the smart MICREAgents will be poured into chemical mixtures, to organize the chemistry from within. Ultimately, such microreactors, like cells in the bloodstream, will open up the possibility of controlling complex chemistry from the inside out.

MICREAgents will provide an unconventional form of computation that microscopically links reaction processing with computation in autonomous mobile smart reactors. This corresponds to a radical integration of autonomous chemical experimentation, a very recent research area, and represents a novel form of computation intertwined with construction. The self-assembling smart micro reactors can be programmed for molecular amplification and other chemical processing pathways, that start from complex mixtures, concentrate and purify chemicals, perform reactions in programmed cascades, sense completion, and transport and release products to defined locations. The project defines a continuous achievable path towards this ambitious goal, making use of a novel pairwise local communication strategy to overcome the limitations of current smart dust and autonomous sensor network communication. It will provide a technical platform spawning research in new computing paradigms that integrate multilevel construction with electronic ICT.

McCaskill's and von Kiedrowski's labs at RUB have already joined forces in previous European Projects forging a path towards artificial cells (PACE, ECCell and MATCHIT). The ECCell project, for example, that finished in February this year, has laid the foundation for an electronic chemical cell. There, the electronics and microfluidics were exterior to the chemistry: in MICREAgents this is being turned inside out. Although these nanoscale structures will soon be sufficiently complex to allow self-replication of their chemical and electronic information, they will not present a proliferative threat to the environment, because they depend for their function on the complex electronic circuit layer that is fabricated as part of their substrate. Self-replication provides for efficient manufacturing of customized smart reagents for specific tasks starting from an affordable mass-produced substrate. It also opens the door to evolvable systems. Computation and construction may become so closely linked that neither will ever be the same again.

The other participants in MICREAgents are teams led by Leroy Cronin (Univ. of Glasgow), Andreas Herrmann (University of Groningen), Itamar Willner (Hebrew University of Jerusalem), Steen Rasmussen (Southern Denmark University), Frantisek Stepanek (Institute of Chemical Technology, Prague), Norman Packard (European Centre for Living Technology), and Peter Wills (University of Auckland). Like the teams at RUB, they are all pioneers in the multidisciplinary areas required to achieve the project goals, with a common grounding in IT.

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