calculations of the energy of each, producing a ranking of the candidates.

The latest challenge, which included a record 25 teams — ten more than the previous contest in 2010 — brought a "massive improvement", says Groom. The molecules selected were "nasty, real-life systems" of the size and complexity to be interesting to drug companies. Previous challenges had included molecules that were flexible or made from multiple parts. This year's challenge combined such features in the same molecules and for one target, asked participants to predict not just one stable structure, but all its many stable forms, known as polymorphs.

PROBLEM SOLVED

The teams rose to the challenge: at the Cambridge workshop, the CCDC announced that each of the five targets, and their polymorphs, appeared in at least one of the shortlists produced by the various methods. A paper with the full results will be published in a special issue of *Acta Crystallographica Section B*.

Moreover, one team, led by Marcus Neumann at the German company Avantgarde Materials Simulation in Freiburg, included the correct solution in each of its shortlists. Had the team combined its efforts with those of a group — led by theoretical chemist Alexandre Tkatchenko at the Fritz Haber Institute in Berlin — that got a perfect score in the ranking phase, the two would together have achieved a perfect score for both rounds and across all targets. Such a result has never occurred in the history of the contest. "With what you have seen from me, and what you have seen from Tkatchenko," says Neumann, "it is fair to claim that to a large extent, this blind test has shown that the problem of organic crystal structure prediction has been solved."

"We have finally kicked the user out of the equation."

More so than in previous blind tests, teams including both Neumann's and Tkatchenko's took into account how quantum mechanical interactions would contribute to the energy of structures. In particular, Tkatchenko used a method published just last year that encompassed these interactions over longer ranges than has been done previously. And Neumann says that his program was unique because it made every decision by itself; most others required human decisions once the computer had returned its calculations. "We have finally kicked the user out of the equation," Neumann says.

Although others agree that the joint feat is a milestone, they stop short of declaring the problem of crystal structure prediction solved. "This does not mean that they would have cracked the problem of predicting all organic crystal structures," says Sally Price, a theoretical chemist at University College London.

And some are frustrated that Neumann has refused to release his computer code: "The day I have a pension plan, I will talk about this freely," he told the workshop. That will make it hard for others to build on his team's breakthrough. "We don't really have a sense of how it works," says challenge participant Claire Adjiman, a chemical engineer at Imperial College London. "But I understand why he doesn't tell us more."

Tkatchenko and Neumann now plan to work together. "My own interest is to understand polymorphism and be able to offer tools to people," says Tkatchenko. "His interest is more commercial, but I'm sure we can find the middle ground."

Both Price and Neumann, meanwhile, are already working with industry on how to use their prediction calculations in drug development. ■

CORRECTION

The News story 'Vaccine gets cautious boost' (*Nature* **526,** 617–618; 2015) incorrectly stated that David Kaslow was involved in the early development of RTS,S.