O.17 (Co)evolutionary methods for predicting exotic compounds and materials with optimal properties

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Until mid-2000s it was thought that crystal structures are fundamentally unpredictable. This has changed, and a special role in this was played by our evolutionary method/code USPEX (http://uspex-team.org). This method can be viewed as a type of artificial intelligence, and routinely allows one to predict stable crystal structures for a given chemical composition], predict all stable compounds formed by given elements, and even predict among all possible compounds the structure and composition that have desired combination of properties. Here I will discuss:

1. Discovery of novel chemical phenomena at high pressure: transparent non-metallic allotrope of sodium, counterintuitive novel sodium chlorides, chemical reactivity of helium, prediction and discovery of new high-temperature superconducting polyhydrides, approaching room-temperature superconductivity.

2. Recent extension of crystal structure prediction to finite temperature, and first results.

3. Development of a new method, Mendelevian search, navigating the chemical space to find the material with desired properties.

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Computational materials discovery:

- Oganov A.R., Saleh G., Kvashnin A.G. (Editors). Computational Materials Discovery. Royal Society of Chemistry. ISBN: 978-1-78262-961-0. (2018).

- Oganov A.R., Pickard C.J., Zhu Q., Needs R.J. (2019). Structure prediction drives materials discovery. Nature Rev. Mater. **4**, 331-348.

USPEX method:

- Oganov A.R., Glass C.W. (2006). Crystal structure prediction using ab initio evolutionary techniques: principles and applications. J. Chem. Phys. **124**, 244704.

- Lyakhov A.O., Oganov A.R., Stokes H.T., Zhu Q. (2013). New developments in evolutionary structure prediction algorithm USPEX. Comp. Phys. Comm. **184**, 1172-1182.

- Kruglov I.A., Yanilkin A.V., Propad Y., Oganov A.R. (2021). Crystal structure prediction at finite temperatures. Submitted.

Mendelevian search:

- Allahyari Z., Oganov A.R. (2020). Coevolutionary search for optimal materials in the space of all possible compounds. NPJ Computational Materials **5**, 55.

Novel high pressure compounds and phases:

- Dong X., Oganov A.R., Goncharov A.F., Stavrou E., Lobanov S., Saleh G., Qian G.R., Zhu Q., Gatti C., Deringer V., Dronskowski R., Zhou X.-F., Prakapenka V., Konopkova Z., Popov I., Boldyrev A.I., Wang H.T. (2017). A stable compound of helium and sodium at high pressure. Nature Chemistry **9**, 440-445.

- Zhang W.W., Oganov A.R., Goncharov A.F., Zhu Q., Boulfelfel S.E., Lyakhov A.O., Somayazulu M., Prakapenka V.B., Konopkova Z. (2013). Unexpected stoichiometries of stable sodium chlorides. Science **342**, 1502-1505.
- Ma Y., Eremets M.I., Oganov A.R., Xie Y., Trojan I., Medvedev S., Lyakhov A.O., Valle M., Prakapenka V. (2009). Transparent dense sodium. Nature **458**, 182-185.
- Semenok D.V., Kvashnin A.G., ..., Troyan I.A., Oganov A.R. (2020). Superconductivity at 161 K in thorium hydride ThH10: synthesis and properties. Materials Today **33**, 36-44.
- Troyan I.A., Semenok D.V., ..., Oganov A.R. (2021). Anomalous high-temperature superconductivity in YH6. Advanced Materials, article 2006832.
- Semenok D.V., Troyan I.A., Ivanova A.G., Kvashnin A.G., Kruglov I.A., Hanfland M., Sadakov A.V., Sobolevskiy O.A., Pervakov K.S., Lyubutin I.S., Glazyrin K.V., Giordano N., Karimov D.N., Vasiliev A.L., Akashi R., Pudalov V.M., Oganov A.R. (2021). Superconductivity at 253 K in lanthanum-yttrium ternary hydrides. Materials Today, in press.