National Science Foundation
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Dear Colleague Letter - Computational and Data-Driven Materials Research (CDMR)

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Computation and the innovative use of data in materials research can drive the discovery of new materials and phenomena, transform research and education, and stimulate the creation of new paradigms for performing materials research. To develop this potential, the Division of Materials Research (DMR) announces a new program, PD 12-8029, *Computational and Data-Driven Materials Research* (CDMR), [1] which offers opportunities distinct from other programs in DMR. For example, simulation, theory, data, and experiment may be combined in a single project to enable a strategic or transformative advance in the fundamental understanding of materials or materials-related phenomena.

CDMR supports materials research driven by computation, data, or theory. Areas of interest include new materials design and preparation, structure development, evolution and control, nanoscale materials, multi-scale properties and optimization across the topical, disciplinary, and interdisciplinary areas represented in DMR programs. Successful projects will advance fundamental understanding of materials or materials-related phenomena through transformative research in which a computational, data-centric, or theoretical activity drives a well-integrated experimental activity or vice versa. Research and education activities supported in this program are distinct from those supported in other programs in DMR in their approach: successful projects will focus more on simulation and less on algorithm development and theory than in the *Condensed Matter and Materials Theory* (CMMT) Program.[2] They may also incorporate experiments and/or a heavy emphasis on data mining. Successful projects may involve the creation of software or databases validated by associated synthesis or experiments to improve theoretical understanding or computational tractability and forge innovative methods to advance the frontiers of materials research. Projects that explore the combination of dedicated computation or data-centric activities with innovative instrumentation leading to transformative tools to advance materials research will also be considered. Projects that create new paradigms for materials research through the innovative use of digital data in ways that complement or dramatically enhance traditional computational, experimental, and theoretical methods to discover new materials or new materials-related phenomena, and advance the fundamental understanding of materials more generally are of particular interest. This program will also support efforts to develop materials research knowledge portals that integrate experimental data with data of simulation or theoretical origin to organize, enhance, and make broadly accessible the digital products of materials research.

CDMR will accept proposals during the window for submitting unsolicited proposals to DMR. As previously announced in PD 12-8029, the next submission window is September 1, 2012 to October 31, 2012 and proposals may be submitted via FastLane or Grants.gov. Additional information about the CDMR program is available on the NSF website at http://nsf.gov/funding/pgm_summ.jsp?pims_id=504827&org=DMR. CDMR will work closely with all other programs in DMR: in particular, CDMR complements the Condensed Matter and Materials Theory (CMMT) Program[2]. CDMR also will accept proposals in response to PD 12-8084, Computational Data-Enabled Science and Engineering (CDS&E)[3]. If there are strong collaborations with industry, please see the Grant Opportunities for Academic Liaison with Industry (GOALI)[4] program solicitation, which can be used in conjunction with this effort 4. Multiple programs may be listed on the proposal cover page, with the most applicable program first.

For questions regarding this new program, CDMR, please contact Dr. Diana Farkas dfarkas@nsf.gov or Dr. Daryl Hess, dhess@nsf.gov. For questions related to the use of FastLane please contact the FastLane Help Desk at fastlane@nsf.gov or telephone 1-800-673-6188. For questions related to the use of Grants.gov please contact Grants.gov support at support@grants.gov or telephone 1-800-518-4726.

Sincerely,

Dr. Ian Robertson
Director, Division of Materials Research

1. CDMR webpage: http://nsf.gov/funding/pgm_summ.jsp?pims_id=504827&org=DMR
2. CMMT webpage: http://nsf.gov/funding/pgm_summ.jsp?pims_id=13623&org=DMR
3. PD 12-8084 http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504813
4. Grant Opportunities for Academic Liaison with Industry (GOALI)
http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf12513&org=NSF