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(Original Signature of Member)

117TH CONGRESS
1ST SESSION

H. R. _____

To provide for a fundamental research program for the application of advanced computing practices to materials science challenges at the Department of Energy, and for other purposes.

IN THE HOUSE OF REPRESENTATIVES

Mr. WEBER of Texas introduced the following bill; which was referred to the Committee on _____

A BILL

To provide for a fundamental research program for the application of advanced computing practices to materials science challenges at the Department of Energy, and for other purposes.

1 *Be it enacted by the Senate and House of Representa-*
2 *tives of the United States of America in Congress assembled,*

3 **SECTION 1. SHORT TITLE.**

4 This Act may be cited as the “Computing Advance-
5 ments for Materials Science Act” or the “CAMS Act”.

1 **SEC. 2. COMPUTATIONAL MATERIALS AND CHEMISTRY.**

2 (a) IN GENERAL.—Section 303 of the Department of
3 Energy Research and Innovation Act (42 U.S.C. 18641)
4 is amended by—

5 (1) redesignating subsections (d) and (e) as
6 subsections (e) and (f), respectively; and

7 (2) inserting after subsection (c) the following:

8 “(d) COMPUTATIONAL MATERIALS AND CHEM-
9 ISTRY.—

10 “(1) IN GENERAL.—The Director shall support
11 a program of fundamental research for the applica-
12 tion of advanced computing practices to foundational
13 and emerging research problems in chemistry and
14 materials science.

15 “(2) COMPUTATIONAL MATERIALS AND CHEM-
16 ISTRY SCIENCE CENTERS.—

17 “(A) IN GENERAL.—In carrying out the
18 activities authorized under paragraph (1), the
19 Director shall select and establish up to four
20 computational materials and chemistry science
21 centers to develop open-source, robust, and vali-
22 dated computational codes and user-friendly
23 software, coupled with innovative use of experi-
24 mental and theoretical data, to enable the de-
25 sign, discovery, and development of new mate-
26 rials and chemical systems including chemical

1 catalysis research and development. These cen-
2 ters shall also focus on overcoming challenges
3 and maximizing the benefits of exascale and
4 other high performance computing systems.

5 “(B) SELECTION.—The Director shall se-
6 lect centers under paragraph (1) on a competi-
7 tive, merit-reviewed basis. The Director shall
8 consider applications from the National Labora-
9 tories, institutes of higher education, multi-in-
10 stitutional collaborations, and other appropriate
11 entities.

12 “(C) DURATION.—A center established
13 under this subsection shall receive support for
14 a period of not more than 5 years, subject to
15 the availability of appropriations.

16 “(D) RENEWAL.—Upon the expiration of
17 any period of support of a center under this
18 paragraph, the Director may renew support for
19 the center, on a merit-reviewed basis, for a pe-
20 riod of not more than 5 years.

21 “(E) TERMINATION.—Consistent with the
22 existing authorities of the Department, the Di-
23 rector may terminate an underperforming cen-
24 ter for cause during the performance period.

25 “(3) MATERIALS RESEARCH DATABASE.—

1 “(A) IN GENERAL.—The Director shall
2 support the development of a web-based plat-
3 form to provide access to a database of com-
4 puted information on known and predicted ma-
5 terials properties and computational tools to ac-
6 celerate breakthroughs in materials discovery
7 and design.

8 “(B) PROGRAM.—In carrying out this
9 paragraph, the Director shall—

10 “(i) conduct cooperative research with
11 industry, academia, and other research in-
12 stitutions to facilitate the design of novel
13 materials;

14 “(ii) leverage existing high perform-
15 ance computing systems to conduct high-
16 throughput calculations, and develop com-
17 putational and data mining algorithms for
18 the prediction of material properties;

19 “(iii) advance understanding, pre-
20 diction, and manipulation of materials;

21 “(iv) strengthen the foundation for
22 new technologies and advanced manufac-
23 turing; and

24 “(v) drive the development of ad-
25 vanced materials for applications that span

1 the Department’s missions in energy, envi-
2 ronment, and national security.

3 “(C) COORDINATION.—In carrying out this
4 section, the Director shall leverage programs
5 and activities across the Department.”.

6 (b) FUNDING.—Out of funds authorized to be appro-
7 priated for the Basic Energy Sciences program of the Of-
8 fice of Science at the Department of Energy, there shall
9 be made available to the Secretary to carry out activities
10 under this subsection \$10,000,000 for each of the fiscal
11 years 2022 through 2031.