{CLAIMS}

1. A material properties prediction system that predicts properties of a material, comprising:

a three-dimensional molecular structure calculation unit having a function of calculating positional coordinates of atoms constituting a molecule from a structural formula of the material;

a spatial structure feature quantity calculation unit having a function of selecting three atoms to form a triangle based on the positional coordinates of the atoms calculated by the three-dimensional molecular structure calculation unit and calculating, as a spatial structure feature quantity, distances between the three atoms and each other atom constituting the molecule; and

a material properties prediction unit that predicts the material properties using the spatial structure feature quantity generated by the spatial structure feature quantity calculation unit,

wherein the material properties prediction unit uses a prediction function to perform the prediction, and the prediction function is obtained by performing regression analysis using the spatial structure feature quantity as the explanatory variable and the properties of the material as an objective variable.

2. The material properties prediction system according to claim 1, further comprising:

an optimal candidate material properties generation unit having a function of searching for a condition for the spatial structure feature quantity such that the material properties to be predicted by the material properties prediction unit satisfy a predetermined standard, and forming a virtual molecular structure from positional coordinates of atoms satisfying the condition.

3. The material properties prediction system according to claim 1,

wherein the spatial structure feature quantity calculation unit selects, as a standard for selecting the three atoms forming the triangle, a combination forming the triangle having the largest area.

4. The material properties prediction system according to claim 1,

wherein the spatial structure feature quantity calculation unit selects a carbon atom as a standard for selecting the three atoms forming the triangle on a priority basis.

5. The material properties prediction system according to claim 1,

wherein when distances between the three atoms and another atom are to be calculated, the spatial structure feature quantity calculation unit calculates the spatial structure feature quantity based on a direction with respect to a formed surface of the triangle while changing signs to be positive and negative.

6. The material properties prediction system according to claim 1,

wherein the spatial structure feature quantity calculation unit defines a circulation direction of the three atoms to select the three atoms forming the triangle.

7. The material properties prediction system according to claim 1,

wherein the spatial structure feature quantity generated by the spatial structure feature quantity calculation unit is stored as a spatial structure feature quantity database, and

the spatial structure feature quantity database includes information identifying the order of the three atoms forming the triangle, distances between the three atoms forming the triangle, and distances between the three

atoms forming the triangle and each other atom constituting the molecule.

8. A computer-implemented information processing method comprising:

performing, by a three-dimensional molecular structure calculation unit, a three-dimensional molecular structure calculation process of receiving a structural formula of a material and calculating positions of atoms constituting a molecule from the structural formula of the material; and

performing, by a spatial structure feature quantity calculation unit, a spatial structure feature quantity calculation process of selecting three atoms to form a triangle based on the calculated positions of the atoms, and calculating distances between the three atoms and each other atom constituting the molecule to obtain a spatial structure feature quantity.

9. The computer-implemented information processing method according to claim 8,

wherein a combination forming the triangle having the largest area is selected as a standard for selecting the three atoms forming the triangle.

10. The computer-implemented information processing method according to claim 8,

wherein a carbon atom is selected on a priority basis as a standard for selecting the three atoms forming the triangle.

11. The computer-implemented information processing method according to claim 8,

wherein a circulation direction of the three atoms is defined to select the three atoms forming the triangle.

12. The computer-implemented information processing method according to claim 11,

wherein when distances between the three atoms and another atom are to be calculated, the spatial structure feature quantity is calculated based on a direction with respect to a formed surface of the triangle while signs are changed to be positive and negative.

13. The computer-implemented information processing method according to claim 8,

wherein the spatial structure feature quantity calculated in the spatial structure feature quantity calculation process is stored as a spatial structure feature quantity database, and

the spatial structure feature quantity database includes information identifying the order of the three atoms forming the triangle, distances between the three atoms forming the triangle, and distances between the three atoms forming the triangle and another atom.

14. The computer-implemented information processing method according to claim 8, further comprising performing, by a material properties prediction unit, a material properties prediction process of predicting the material properties using, as an explanatory variable, the spatial structure feature quantity calculated in the spatial structure feature quantity calculation process,

wherein the material properties prediction process uses a prediction function to perform the prediction, and the prediction function is obtained by performing regression analysis using the spatial structure feature quantity as the explanatory variable and the material properties as an objective variable.